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Final Report: Request for Symposia Support: Switchable Catalysis

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5f. WORK UNIT NUMBER

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Boston College
140 Commonwealth Avenue

Chestnut Hill, MA 02467 -3800

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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES)
U.S. Army Research Office
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Approved for public release; distribution is unlimited.

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The views, opinions and/or findings contained in this report are those of the author(s) and should not contrued as an official Department of the Army position, policy or decision, unless so designated by other documentation.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Jeffery Byers
UU	UU	UU	UU		19b. TELEPHONE NUMBER 617-552-3605

RPPR Final Report
as of 03-Jan-2019

Agency Code:

Proposal Number: 70397CHCF **Agreement Number: W911NF-17-1-0139**
INVESTIGATOR(S):

Name: Jeffery Byers
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Organization: **Boston College**
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Country: USA
DUNS Number: 045896339 EIN: 042103545
Report Date: 30-Jun-2018 Date Received: 06-Dec-2018
Final Report for Period Beginning 01-Apr-2017 and Ending 31-Mar-2018
Title: Request for Symposia Support: Switchable Catalysis
Begin Performance Period: 01-Apr-2017 **End Performance Period:** 31-Mar-2018
Report Term: 0-Other
Submitted By: Jeffery Byers Email: jeffery.byers@bc.edu
Phone: (617) 552-3605
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: 0 **STEM Participants:** 0

Major Goals: The major goal of the grant was to gather leaders and emerging scientists in the area of switchable catalysis in a symposium held at the 253 American Chemical Society National Meeting held on April 2-6, 2017. The purpose for this gathering was so that researchers could share new results with each other in order to foster new relationships and build the community of scientists studying switchable catalysis.

Accomplishments: There were 29 speakers and 13 poster presenters at the symposium. The presenters disseminated new ideas and new collaborations were established that have driven the field forward in new and exciting directions. Since the symposium, which was the first one ever devoted to this topic, several high impact papers emerged along with several reviews in the general area. New collaborations were established that will likely lead to exciting advances in the field in the coming years.

Training Opportunities: Nothing to Report

Results Dissemination: Nothing to Report

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Jeffery A Byers
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

RPPR Final Report
as of 03-Jan-2019

Participant Type: Co PD/PI
Participant: Paula Diaconescu
Person Months Worked: 1.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Final Report: "Switchable Catalysis", Symposium Support

A. Location and Dates

"Switchable Catalysis", 53rd American Chemical Society National Meeting and Exposition on April 2-3, 2017 in San Francisco, CA.

B. Summary

Switchable catalysis is an atom-economical method that generates multiple, catalytically active species with different reactivity. Because these species originate from a single precursor and are readily controlled by the external stimuli, rapid production of molecular complexity is achieved and chemical synthesis is made more efficient and less costly. The topics that were covered by participants included photo-switchable, redox-controllable, pH-responsive, ion selective, and host-guest recognition reactions, which have led to significant advances that have made controlling chemical reactions with switchable catalysis possible. The applications for this emerging technology are broad and particularly relevant to environmental chemistry including applications in energy science from renewable resources, degradable polymers, and green chemistry. The speakers who presented (see list below) were diverse and international featuring male and female speakers, scientists at all career levels, and speakers from all over the world. Moreover, speakers with different chemical backgrounds (organic, inorganic, and polymer chemists) were purposely chosen in order to create a forum that fosters the exchange of new ideas across multiple disciplines. In addition to the two-day symposium, the lectures were complemented by a poster session, which was comprised of student and postdoctoral researchers (see list below) in order to offer career opportunities to the next generation of scientists in the field. To further foster the exchange of ideas and the development of new and lasting relationships, a symposium dinner was held for all participants.

C. Topics Covered

- Redox-switchable polymerization catalysis
- Photoredox catalysis and its application in organic synthesis
- Using molecular recognition to control catalytic reactions
- Computational investigations into the origin of switchable reactions
- Controlling polymer patterning using switchable catalysts
- Controlling hierarchichal structures using switchable polymerization catalysis
- pH responsive catalysts for energy applications

D. Outcomes/Impact

Participants in the symposium disseminated new ideas and new collaborations were established that have driven the field forward in new and exciting directions. Since the symposium, which was the first one ever devoted to this topic, several high impact papers emerged along with several reviews in the general area. New collaborations were established that will likely lead to exciting advances in the field in the coming years.

E. Participants

Speakers:

1. Chris Bielawski, Ulsan National Institute of Science and Technology, Korea
2. Andrew J. Boydston, University of Washington

3. Jeff Byers, Boston College (**PI, co-chair**)
4. Frank Breher
5. Thibault Cantat, CEA, France
6. Jean-François Carpentier, University of Rennes, France
7. Changle Chen, University of Science and Technology of China
8. Eugene Chen, Colorado State University
9. Paul Chirik, Princeton University
10. Christopher Cramer, University of Minnesota
11. Donald Darensbourg, Texas A&M University
12. Paula Diaconescu, University of California, Los Angeles (**co-chair**)
13. Natalie Fey, University of Bristol
14. Brett Fors, Cornell University
15. Etsuko Fujita, Brookhaven National Lab
16. Brian Long, University of Tennessee
17. Kazushi Mashima, Osaka University
18. Krzysztof Matyjaszewski, Carnegie Mellon University
19. Parisa Mehrkhodavandi, University of British Columbia, Canada
20. Chad Mirkin, Northwestern University
21. David Nicewicz, The University North Carolina at Chapel Hill
22. Jun Okuda, RWTH Aachen, Germany
23. Javier Read de Alaniz, University of California, Santa Barbara
24. Michael Reynolds, Shell
25. Mitsuo Sawamoto, Kyoto University, Japan
26. Alex Spokoyny, University of California, Los Angeles
27. Corey Stephenson, University of Michigan
28. Charlotte Williams, Imperial College, UK
29. Tehshik Yoon, Wisconsin University

Poster presenters (13 participants):

Kayla Delle Chiaie, Stephanie Quan, Arnaud Thevenon, Rongjia Zhang, Jeffrey Kehl, Junnian Wei, Amy Lai, Soohik Ro, Madeline Riffel, Ruxi Dai, Theresa Williams, Mark Abubekerov, Yi Shen.

ACS Chemistry for Life®

253rd American Chemical Society National Meeting & Exposition

April 2-6, 2017 • San Francisco, CA

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Download the ACS San Francsico Mobile App or access the Digital Meeting Program

at www.acs.org/SanFran2017 for up-to-date meeting information.

www.acs.org/meetingapp

ANDROID APP ON Google play | Available at amazon | Available on the App Store

*Online version is also available for internet enabled devices

253rd American Chemical Society National Meeting & Exposition

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- **Hilton San Francisco Union Square, Nob Hill 1:** 415-923-7550
- **Hotel Nikko San Francisco, Lincoln Boardroom:** 415-403-1813
- **InterContinental San Francisco, Mission Room:** 415-616-6576
- **Marriott Union Square, City Suite:** 415-398-8900 x7519
- **San Francisco Marriott Marquis, Willow:** 415-284-8053
- **San Francisco Marriott Marquis, Awards Office, Laurel:** 415-284-8013
- **Moscone Center, South Lobby:** 415-978-3600
- **Moscone Center/West Building, Lobby:** 415-348-4400
- **Parc 55 San Francisco, Davidson:** 415-403-6670
- **Park Central San Francisco, Press Room:** 415-618-6812

INFORMATION CONTACTS

- **Attendee Registration, Moscone Center, North Lobby**: 415-978-3609
- **Career Fair Information Center, Moscone Center, Halls B/C**: 415-978-3613
- **Exhibitor Registration, Moscone Center, South Lobby**: 415-978-3611
- **Finance Office - Moscone Center, Room 110**: 415-978-3608
- **Host Local Section Booth, Moscone Center, North Lower Lobby**: 415-978-3616
- **Housing Assistance, Moscone Center, North Lobby**: 415-978-3610
- **Member Services, Moscone Center, North Lobby**: 415-978-3615
- **Press Center, Moscone Center, South Lobby**: 415-978-3605
- **Shuttle Desk Moscone Center, Outside West Lobby**: 415-348-4406
- **Society Program Office, Mason Room**: 415-923-7551
- **Governance Office, Union Square 22**: 415-923-7549

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Fax: 202-872-4615 E-mail: help@acs.org Website: www.acs.org

The American Chemical Society is a self-governed individual membership organization of members at all degree levels and in all fields of chemistry. The Society provides a broad range of opportunities for peer interaction and career development, regardless of professional or scientifc interests. The programs and activities conducted by ACS today are the products of a tradition of excellence in meeting member needs that dates from the Society's founding in 1876.

This On-site Meeting Program is published by the American Chemical Society as a service to its attendees. Information contained herein is subject to change without notice. While every effort is made to ensure accuracy, ACS makes no warranties, expressed or implied, related to the information. For the official technical program for the 253rd National Meeting & Exposition, refer to www.acs.org/sanfran2017. All San Francisco photos in this program are courtesy of the San Francisco Convention and Visitors Bureau and Shutterstock.

ACS Chemistry for Life®

Welcome to San Francisco and the 253rd ACS National Meeting

Welcome to beautiful San Francisco for the 253rd ACS National Meeting. It is my pleasure to join all of you in this vibrant city, and a favorite location for our meetings.

Advanced Materials, Technologies, Systems & Processes is the theme of this meeting. Twenty nine technical divisions and six committees are hosting original programming, including 1,100 half-day oral sessions and 144 poster sessions. More than 14,500 papers and nearly 5,700 posters will be presented at the meeting. In addition to symposia, there are a number of special events planned throughout the week.

Allison A. Campbell
ACS President

There are three Presidential Symposia that I encourage you to attend, as well as 14 symposia that I am recommending. Organized by the Division of Professional Relations, the LGBT Graduate & Postdoctoral Student Chemistry Research Symposium on Sunday and Monday will include scientific talks by LGBT graduate and postdoctoral students and a panel discussion on issues that affect LGBT students (Hotel Nikko San Francisco, Nikko Ballroom III). Sunday afternoon, Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal will assess the progress made in critical areas of chemistry since first highlighted in a 1995 issue of the journal (San Francisco Marriott Marquis, Golden Gate A). On Monday, Science for a Sustainable Energy Future will focus on scientific advances in energy storage and chemical and biological approaches to energy conversion (Moscone Center, Room 133).

On Sunday afternoon, please join your colleagues at noon for the ACS Board of Directors Regular Session as we hear from two renown guest speakers: Joseph M. DeSimone presenting on the Future Fabricated with Light: The Launching of Carbon, and Anne Milasinic Andrews, talking about The Brain is More Than a Computer (Moscone Center, Gateway Ballroom 103/104).

On Monday afternoon, Bradley D. Olsen from the Massachusetts Institute of Technology will present the Kavli Foundation Emerging Leader in Chemistry Lecture on Classical challenges in the physical chemistry of polymer networks. Following his presentation, Jennifer A. Doudna of the University of California, Berkeley will give the Fred Kavli Innovations in Chemistry Lecture on CRISPR systems: Nature's toolkit for genome engineering (Moscone Center, Gateway Ballroom 103/104).

Throughout the meeting, many education-focused programs for high school teachers, undergraduate and graduate students, postdocs, and chemical professionals will be offered. For job seekers and employers, the career fair will feature on-site interviews, one-on-one career assistance, and workshops. Please find time to walk the expo hall where more than 400 booths will showcase services, instruments, books, and lab equipment of more than 250 companies.

My personal thanks to the members of the Santa Clara Valley Section and California Section; the divisional program chairs and symposium chairs responsible for organizing the technical sessions; and the ACS staff for making it all happen. Thanks to you for contributing to the success of this meeting, and of course for attending.

Allison A. Campbell
ACS President

Welcome Message from Kathryn Beers, San Francisco Thematic Program Chair

The Spring 2017 ACS National Meeting will be held April 2–6 in San Francisco, CA. The theme for the meeting is Advanced Materials, Technologies, Systems, and Processes.

Kathryn Beers
San Francisco Thematic Program Chair

The plenary session on Sunday afternoon, April 2, includes four invited lectures: Dr. Peter Green (National Renewable Energy Laboratory) will discuss "Clean energy challenge: An integrated approach involving basic research, innovation and human factors;" Dr. Jeffrey Linhardt (Verily Life Sciences) will discuss "Technology at the interface of microelectronics, life sciences, and big data: Materials challenges;" Dr. Ann-Christine Albertsson will discuss "From design and synthesis to advanced properties and sustainable polymeric materials;" Dr. Keith Watson (The Dow Chemical Company) will discuss "Fostering industrial and academic partnerships."

The Kavli Foundation Lecture Series will be held Monday, April 3. The Kavli Foundation Emerging Leader in Chemistry Lecture by Prof. Bradley Olsen (Massachusetts Institute of Technology) on "Classical challenges in the physical chemistry of polymer networks" and the Fred Kavli Innovations in Chemistry Lecture by Dr. Jennifer Doudna (UC Berkeley, Lawrence Berkeley National Lab) on "CRISPR systems: Nature's toolkit for genome engineering".

The technical program constructed by the ACS divisions includes 134 symposia that support the theme of the meeting. Divisions and committees with symposia supporting the theme include AGFD, ANYL, BIOT, CATL, CELL, CHED, CINF, COLL, COMP, ENFL, ENVR, HIST, I&EC, INOR, NUCL, ORGN, PHYS, PMSE, POLY, SCHB, and YCC. MPPG is cosponsoring a total of 27 symposia.

The program for the meeting and other information is available online at the website of the meeting, www.acs.org/sanfran2017.

I am very grateful to the members of the local section, the program chairs of the divisions and committees listed above, the thematic symposia chairs, and the ACS staff for their work in supporting the theme of this meeting. I look forward to meeting you in San Francisco!

Kathryn Beers
Thematic Program Chair

OFFICE OF THE GOVERNOR

April 2, 2017

American Chemical Society

On behalf of the State of California, I am pleased to welcome you to the 253rd American Chemical Society (ACS) National Meeting & Exposition.

Since its inception in 1876, the ACS has supported chemists and the chemical enterprise by providing professional and academic support to a growing network of members. Scientific research and emerging technologies continue to spur economic growth in California and in the broader global community. I commend all those who have come together to discuss the power of chemistry and I applaud your efforts to foster the innovators and innovations of tomorrow.

Best wishes for a memorable and productive meeting.

Sincerely,

EDMUND G. BROWN JR.

Office of the Mayor
City & County of San Francisco

Edwin M. Lee

GREETINGS FROM THE MAYOR OF SAN FRANCISCO

On behalf of the City and County of San Francisco, it is my pleasure to welcome you to the 253rd National Meeting of the American Chemical Society, focused on *Advanced Materials, Technologies, Systems and Processes*, held on April 2-6, 2017

The American Chemical Society (ACS) is the world's largest scientific society and one of the world's leading sources of authoritative scientific information. ACS is at the forefront of the evolving worldwide chemical enterprise and the premier professional home for chemists, chemical engineers and related professions around the globe.

San Francisco is proud to host this valuable event as our City continues to be a leader in scientific innovation, and we welcome the gathering of the brightest minds in the chemical sciences.

Congratulations to the American Chemical Society for their dynamic and visionary commitment to improving the lives of others through the transforming power of chemistry. I commend all the individuals who helped make this event a true success, and I wish you all the best in your future endeavors!

With warmest regards,

Edwin M. Lee
Mayor

1 Dr. Carlton B. Goodlett Place, Room 200, San Francisco, California 94102-4641
(415) 554-6141

GENERAL MEETING INFORMATION

YOUR MEETING REGISTRATION entitles you to a range of programming, including scientific sessions, invited symposia, poster sessions, special lectures and events, award presentations, workshops, and the exposition. Interact with chemical scientists from around the world by participating in social events, networking opportunities, exhibitor sessions, and educational activities, with many events offered at no additional charge. Certain workshops, short courses, and ticketed events require a separate entry fee, as indicated in this program.

REGISTRATION

All attendees, including speakers and poster presenters, must register for the meeting to participate in the technical sessions. Sponsored speakers should contact their symposium organizer or division program chair to clarify the terms of their invitation and to determine who will complete the speaker's registration. Attendees must display their badge at all times for admission to all official ACS sessions and events.

Early registration. U.S. residents who registered by February 20 received their badge credentials by mail. International registrants (this includes Canada and Mexico) must pick up their badge credentials at ACS Attendee Registration.

Standard & on-site registration. Attendees who registered after February 20 must pick up their badge credentials on-site.

Registration changes. Attendees can modify their existing registration or generate a receipt from the registration website by following the instructions in their confirmation message. Attendees can also contact the ACS National Meeting Registration Center or update their registration on-site at ACS Attendee Registration. Bring your confirmation and/or badge credentials with you to the meeting for faster processing.

Registration methods. All registrants received a confirmation via the original method of registration.

Internet. Register online at www.acs.org/sanfran2017 until April 6. A valid credit card is required to register online, and online registrations are real-time transactions.

Telephone. Call the ACS National Meeting Registration Center at 800-251-8629 (U.S./Canada only) or 508-743-0192 (international), Monday through Friday, 9:00 AM to 5:00 PM ET.

Fax/mail. Submit the registration form via fax by April 6 at 508-743-9604, or mail it to ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532.

On-site. Register during the meeting at ACS Attendee Registration at standard registration rates. ACS Attendee Registration will be open at the Moscone Center, North Lobby, on Saturday, 3:00 to 6:00 PM; Sunday, 7:30 AM to 7:30 PM; Monday, 7:30 AM to 9:00 PM; Tuesday, 7:30 AM to 5:00 PM; Wednesday, 7:30 AM to 4:00 PM; and Thursday, 7:30 AM to 1:00 PM.

REGISTRATION PAYMENTS. Registration fees can be paid by check, money order, credit card (American Express, Discover, MasterCard, or VISA), or bank wire transfer. Make checks payable in U.S. dollars to the American Chemical Society, and include a completed registration form with each payment. Registration fees should not be combined with any other payment (such as membership dues). Purchase orders and training requests are not accepted. For wire transfer payments, contact the ACS Finance Department at 202-872-6106 or e-mail bankwires@acs.org. **Registration forms received without payment will not be processed.**

REGISTRATION ASSISTANCE. The ACS National Meeting Registration Center will be available from 9:00 AM

MEETING INFO ON THE WEB

Registration, housing, technical programming, special events, participating exhibitors, and other meeting details are available at www.acs.org/sanfran2017.

BADGES

All attendees are required to wear their badges for all technical sessions, poster sessions, and other official meeting events. Our badge holders are recyclable and biodegradable. Please discard appropriately.

REGISTRATION CATEGORY	FEE EARLY BY FEB. 20	FEE STANDARD FEB. 21
MEMBERS		
ACS affiliate	$445	$535
Postdoctoral member	445	535
Emeritus or retired member	225	270
50-year member	No fee	No fee
Unemployed member (Dues waiver required)	No fee	No fee
Precollege teacher	110	110
Graduate student	225	225
Undergraduate	110	110
One-day registrant	225	270
NONMEMBERS		
Chemical scientist	$780	$935
Postdoctoral scientist	780	935
Visitor: Nonchemical scientist or chemical technician	445	535
Precollege teacher	110	110
Graduate student	445	445
Undergraduate	225	225
One-day registrant	445	535
Guest of registrant*	45	45
EXPOSITION-ONLY VISITORS		
Adult, exposition only	$60	$60
Student, exposition only	30	30

* Registration is restricted to a spouse or family member of registered attendee having no affiliation with the field of chemical science and who is not eligible to become an ACS member. Only one guest registration is allowed per registering attendee, and the guest registration must be completed and paid by the registering attendee at time of original registration.

ACS BADGE REPRINT POLICY

1st badge reprint: no charge, upon proper identification and confirmation of registration payment, a duplicate badge is issued.
2nd badge reprint: attendee completes a duplicate badge request, shows identification (which we copy), a charge of $25 is paid (cash/credit card), a duplicate badge is issued.
3rd badge reprint: attendee completes a duplicate badge request, shows identification (which we copy), a charge of $50 is paid (cash/credit card), a duplicate badge is issued.
For any badge beyond the 3rd: attendee completes a duplicate badge request, shows identification (which we copy), a charge of $100 is paid (cash/credit card), a duplicate badge is issued.

to 5:00 PM ET by telephone, fax, mail, or e-mail. Service representatives can be reached by phone at 800-251-8629 (U.S./Canada only) or 508-743-0192 (international), by fax at 508-743-9604, by e-mail at acs@xpressreg.net, or by mail at ACS Registration, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532.

Registration cancellations/refunds. All cancellations and refund requests must be submitted in writing by March 6 to guarantee the registrant a full refund less a $50 administrative fee. Refund requests made after March 6 will not be honored. Your registration badge credentials and a copy of your registration confirmation must be attached to your request. All refunds will be issued via the original payment method, and refunds will be processed within 30 days after the meeting. Send your request to ACS Registration Cancellation, c/o CDS, 107 Waterhouse Rd., Bourne, MA 02532, or fax it to 508-743-9604 (save your fax confirmation sheet).

ONSITE PROGRAM BOOK NO LONGER FREE

Copies of the on-site program book will be available for $10 until February 20 through the online registration process. The standard fee of $20 will apply after February 20. In response to numerous requests, the author index will be included in the printed program booklet. Satellite registration and on-site program purchase/pickup locations will be located at the Moscone Center, North Lobby; Hilton Union Square, West Lounge; and Grand Hyatt San Francisco, Theater Level. Credit cards, debit cards, and checks will be accepted at these locations. We encourage meeting attendees to download the ACS San Francisco mobile app or access the ACS San Francisco digital meeting program with author index in early April. These digital options will provide quick access to the full technical program, along with special features so you can easily build your schedule.

Social event ticket cancellations/refunds. Social event cancellations received by March 6 entitle the registrant to a full refund. Refund requests made after March 6 will not be honored. Event tickets and a copy of your registration confirmation must be attached to your request.

Abstract cancellations/refunds. Abstract USB flash drives (thumb drives) and their shipping costs are nonrefundable.

MEMBER REGISTRATION. You must enter a valid ACS membership number during registration to register as a member and receive your ACS member discount on registration fees. Your registration options will automatically appear in accordance with your current membership status in the ACS membership database. Your ACS membership number can be found on your ACS membership card or your *Chemical & Engineering News* address label. Address questions about your membership status to ACS Member Services at 800-333-9511 (U.S./Canada only) or 614-447-3776 (international) or by e-mail at service@acs.org.

NONMEMBER REGISTRATION. Save money on discounted registration fees by joining ACS. You can join ACS now through the online ACS membership application at www.acs.org/join or by contacting ACS Member Services and then registering for the meeting at your member rate. To receive your meeting discount, you must join the society before you register for the meeting. New memberships or questions about membership status should be handled through ACS Member Services at 800-333-9511 (U.S./Canada only) or 614-447-3776 (international) or by e-mail at service@acs.org.

PRESS/MEDIA REGISTRATION. Press registration is complimentary for credentialed members of the news media who are approved by the ACS Office of Communications (restricted to reporters and editors working full-time for print or broadcast news). Press badges may be picked up with valid media credentials from the Press Room at the Moscone Center. For more information, visit www.acs.org/pressroom.

EXPO-ONLY ADMISSION. All meeting attendees with a valid badge receive complimentary admittance into the exposition as part of their registration. Individuals who want to visit the exposition without registering for the meeting's technical sessions can register for an expo-only adult badge for $60 or $30 for students with school identification. Register online or in person at ACS Attendee Registration.

EXHIBITOR REGISTRATION. Exhibitor registration is handled exclusively through ACS National Expositions at www.acs.org/expositions.

CAREER FAIR EMPLOYER REGISTRATION. ACS Career Fair Employer registration is handled exclusively through ACS Careers at www.acs.org/careers.

ACCOMMODATIONS

CONFERENCE DIRECT is the official housing bureau for the ACS National Meeting in San Francisco. ACS does not endorse booking hotel reservations through any other sources. All attendees who made their reservation through ConferenceDirect will receive complimentary internet access in their sleeping rooms and will be automatically entered in the ACS Housing Drawing.

ON-SITE HOUSING. An onsite housing desk will be available during the meeting in the registration area of the Moscone Convention Center to assist with last-minute housing changes or needs.

RESERVATION. All registrants received confirmation for reservations made directly through ConferenceDirect. Each confirmation contains a unique number that is proof of your reservation through ConferenceDirect.

Published ACS rates apply to hotel stays from March 28 – April 8. To extend your stay beyond these dates, you must reserve additional nights directly through the hotel.

ACS GREENER MEETINGS

The ACS Department of Meetings & Expositions Services and the Committee on Meetings & Expositions are committed to greener meetings. For each national meeting, we collaborate with the destination city, the convention center, and our hotel and vendor partners to reduce our environmental footprint and raise the bar for industry sustainability practices.

Interested in learning more about how we're leading the way? Go to www.acs.org/greenermeetings to read about our greener meeting initiatives and access our annual Event Sustainability Report.

For its efforts, ACS has been recognized as a cowinner of the 2016 UFI Sustainable Development Award. Here are a few reasons why:

- ACS seeks sustainable convention center venues to track energy, waste, and water data for each meeting.
- ACS offsets staff event emissions in partnership with American Forests (over 16,000 trees planted since 2014) and shuttle emissions in partnership with Transportation Management Services (TMS) and carbonfund.org. In 2016, ACS and its partners indirectly offset 3,270 metric tons of CO_2.
- ACS engages hotel partners to survey and collect information on sustainability initiatives and perform on-site walkthroughs of hotel room block properties to encourage hotels to increase sustainability efforts and validate said efforts. These sustainability initiatives are provided to meeting attendees through the Hotel Sustainability Green Grid, published on the ACS housing page. ACS collaborates with catering partners to bring as many local food items to all food and beverage functions during the meeting.

TAKE THE ACS GREENER MEETINGS PLEDGE. In 2016, 13,842 meeting attendees took the Greener Meetings Pledge, representing 47% of total attendees. As a result of attendee donations through American Forests, 3,714 trees were planted. Do your part and take the Greener Meetings Pledge during registration!

I pledge to:

- Take advantage of linen reuse initiatives at my hotel, turn off the lights when away from my room, and participate in any incentive programs for declining housekeeping service during my stay, such as Starwood's Make a Green Choice program.
- Responsibly dispose of recyclable materials (paper, plastic, glass, aluminum) in the Moscone Center and hotels.
- Use the meeting mobile app and digital program instead of the printed on-site program.
- Enjoy the city, burn calories, and reduce my carbon footprint by walking to and from my hotel.
- Use the ACS carbon-offset shuttle service provided by TMS when walking isn't an option.
- Bring a reusable water bottle to avoid the cost and waste associated with disposable, petroleum-based plastic water bottles.

Suggestions? Send them to the ACS Committee on Meetings & Expositions at greenermeetings@acs.org.

TRAVEL & TRANSPORTATION

TRANSPORTATION DISCOUNTS. ACS has negotiated special travel discounts with the following partners. To get the best rates and avoid service fees, we recommend making reservations online (except for Amtrak).

AIRLINES:
Delta
delta.com/meeting; 800-328-1111
Discount code: NMPBR
United Airlines
united.com; 800-426-1122
Discount code: ZXMC508834

TRAIN:
Amtrak
800-872-7245
Discount code: X90C-958
(phone reservations only)

CAR RENTAL:
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avis.com; 800-331-1600
Discount code: B923099
Hertz
hertz.com; 800-654-2240
Discount code: 02UZ0016

AIRPORT GROUND TRANSPORTATION. San Francisco International Airport is located 13 miles south of downtown San Francisco.

Public transportation. San Francisco has a comprehensive public transportation system that includes the Bay Area Rapid Transit (BART) system, Caltrain commuter rail, and SamTrans public bus service. For more information please visit bit.ly/2jueoyY.

Taxi services. Taxis depart from the designated taxi zones located at the roadway center islands on the arrivals and baggage claim level. Fares range from $46.16–$66.16. A $2.00 exit surcharge is included in all San Francisco taxicab meter fares for rides originating from San Francisco International Airport.

TRAVELING TO MEETING VENUES. The Moscone Center is located at 747 Howard St., San Francisco, CA 94103.

ACS shuttle. Complimentary shuttle service will be provided between the Moscone Center and official ACS hotels, with the exception of hotels within walking distance.

Parking. There is no parking provided at the Moscone Center for attendees or exhibitors. Nearby parking garages are listed on the Moscone Center website.

ACS MEMBER SERVICES

ACS MEMBER SERVICES. ACS staff can assist you on-site with joining ACS, renewing memberships, completing adjustments to member records, and answering general membership questions. ACS members receive discounted rates when registering for the meeting.

ACS Member Services is located in the North Lobby near attendee registration in the Moscone Center and is open Saturday, April 1, 3:00 to 6:00 PM; Sunday, April 2, 7:30 AM to 7:30 PM; Monday, April 3, 7:30 AM to 9:00 PM; Tuesday, April 4, 7:30 AM to 5:00 PM; Wednesday, April 5, 7:30 AM to 4:00 PM; and Thursday, April 6, 7:30 AM to 1:00 PM.

ONLINE SOCIAL NETWORKING TOOLS. Start discussions and connect with other attendees at the ACS Network and the ACS Facebook page. Follow ACS national meetings on Twitter. Read, comment on, and share C&EN's coverage of ACS meetings.

ATTENDEE NATIONAL MEETING E-NEWSLETTER. Receive official updates on ACS national meetings, including locations, registration and accommodation dates, information and discounts, resources, and event details. You can sign up and manage your subscriptions with your free ACS ID. E-mail meetingnews@acs.org to subscribe.

BUSINESS CENTER. The Moscone Business Center provides full service business needs for your convenience, including photocopying, faxing, computer workstations, and printing services. Shipping is provided through UPS. Office supplies and souvenirs are also available for purchase.

MEMBER INSURANCE PROGRAM. Do you need help in determining the right amount of financial protection for you and your loved ones? Are you confused about how to plan for your family's financial future? Do you have student debt or a mortgage? Visit the ACS Member Insurance kiosk at exposition booth 725 and learn how we can help you protect the elements you've built your life around with plans ranging from Life & Health Insurance, International Term Life, Auto & Homeowners Plus, Disability Income, Long-Term Care, Professional Liability, and more. Also learn about our latest addition: Chemical Educators' Legal Liability.

If you are a chemistry educator, visit us for a complimentary 15-minute consultation about Chemical Educators' Legal Liability, and learn how this policy provides the unique coverage necessary for you. Visit haysconsult.setmore.com to schedule your complimentary consultation.

To learn more about the insurance plans available to you, visit www.acs.org/insurance

ON-SITE MEETING ARRANGEMENTS

ADA-COMPLIANT MEETING. The Moscone Center provides service ramps to entrances and elevated areas, braille instructions and directions throughout the building, and pay phones on each level of the facility with (TDD) hearing-impaired functions. More information is available at moscone.com.

ACS is dedicated to ensuring that no individual with a disability is excluded, denied services, segregated, or otherwise treated differently because of the absence of auxiliary aids and services identified in the Americans with Disabilities Act. If you require special accommodations to participate in the meeting, communicate your needs to ACS Meeting Services by e-mail at nationalmeetings@acs.org, by fax at 202-872-6128, or by phone at 202-872-6111 by February 20 to allow enough time to fulfill your request. Keep in mind that ACS may not be able to accommodate last-minute requests.

If you have an emergency or need immediate assistance during the meeting, contact any ACS Operations Office.

ASSISTANCE. Our greeters will be positioned throughout the meeting and can help you navigate the on-site program, find a particular session or room, and answer questions. Lost-and-found items at the convention center should be directed to the ACS Operations Office located in the South Lobby. Messages left at the ACS Operations Office will be conveyed to attendees via the Meeting Mail system, but ACS cannot accept responsibility for the delivery of any messages, mail, or packages.

ATTENDEE BADGES. Attendees and guests must be registered and display their badges at all times to be admitted to all official ACS sessions and events.

ATTENDEE MESSAGING/MEETING MAIL. After registering for the meeting, you will be assigned a temporary electronic mailbox to exchange personal messages with other registered attendees via Meeting Mail. Meeting Mail will be available before, during, and after the meeting at www.acs.org/sanfran2017. Use the Meeting Mail terminals located in the Moscone Center. Telephone messages left at the ACS Information Booths will be conveyed to attendees via the electronic message center, but the society cannot accept responsibility for the delivery of any messages. No one will be paged in meeting rooms.

AUDIO TAPING, PHOTOGRAPHY & VIDEOTAPING. The use of any device to capture images (e.g., cameras and camera phones) or sound (e.g., tape and digital rebroadcast) of speakers or presentations is strictly prohibited at all ACS meetings and events without express written consent from ACS.

CHILD CARE. Camp ACS will be available to all meeting attendees free of charge from 7:00 AM to 6:00 PM on Sunday, April 2, through Thursday, April 6. At Camp ACS, children two (and potty-trained) to 16 years of age can participate in age-appropriate activities, including arts and crafts and active games, while you enjoy the meeting. For your child's safety, the location of Camp ACS will not be communicated until your registration is confirmed. On-site registration will be accepted on a space-available basis.

ELECTRONIC DEVICES. As a courtesy to other meeting attendees, electronic devices must be operated in silent or vibrate mode in technical or educational sessions. Cell phone conversations are not permitted in meeting rooms.

EMERGENCIES DURING ACS MEETING EVENTS. ACS will place detailed instructions in each meeting room to be used if an emergency occurs during an ACS meeting event. These instructions will

TIPS FOR A SAFE STAY IN SAN FRANCISCO

- Be aware of your surroundings at all times.
- Don't wear your meeting badge outside the convention center or hotels.
- Don't wear fancy jewelry or carry expensive technology in plain sight.
- Carry your briefcase, tote bag, purse, or laptop carrier close to your body.
- Don't leave valuables in your hotel room. Get a hotel safe deposit box.
- Walk in open and well-lit areas at night.
- Travel in groups. Don't be a loner, particularly in the evening.
- Use common sense. If someone or someplace looks suspicious, report it and/or avoid it.
- If an emergency occurs during a meeting event, refer to detailed instructions placed by ACS staff inside each meeting room to follow in case of emergencies. Report emergencies to the nearest security guard or to any ACS Operations Office during the meeting.
- If an emergency occurs outside an ACS event, contact police or emergency assistance by dialing 911 or seeking assistance from the facility where the emergency has occurred.
- Should a catastrophic event occur while the meeting is under way, follow safety and security instructions issued by the facility where you are located at the time of the event.

revolve around following the established emergency guidelines of the facility where the emergency occurs. Report emergencies to the nearest security guard or to any ACS Operations Office during the meeting. Should a catastrophic event occur, attendees should follow safety and security instructions issued by the facility where they are located at the time of the event.

HOST LOCAL SECTION. ACS gratefully acknowledges the cooperation and assistance of the ACS California and Santa Clara Valley Local Sections and their members in handling local arrangements. Volunteers have planned many interesting activities; the Host Local Sections booth will be located in the Lower North Lobby.

INTERNATIONAL REGISTRANTS. Many international visitors are required to hold a visa prior to being admitted to the U.S. because of security measures in place at airports and other border crossings. All visa applicants are advised to apply for their visa in their home country as soon as possible. Detailed information for international attendees can be found at www.acs.org/sanfran2017.

INTERNET & COMPUTER SERVICES. Use our electronic communication services before, during, and after the meeting. Once you get to the meeting, you can access your e-mail and the internet as well as your personal Meeting Mail mailbox from Meeting Mail terminals, which will be located throughout the Moscone Center.

LITERATURE & PRODUCT DISTRIBUTION. Promotions, posters, and literature distribution by attendees, exhibitors, or other groups during the meeting must be done within their own contracted meeting space or exhibit booth and not in public meeting space, with the exception of designated marketing opportunities. No one is authorized to place any promotional items in public meeting space except the ACS Operations Office at a given location. Items left in violation of this policy will be removed and discarded. Literature distribution at specific division tables is under the control of that division, and permission must be secured from the division before placing any items on its table.

LUGGAGE & COAT CHECK. A luggage and coat check station will be available during registration hours from Sunday through Thursday in the North Lobby. Items left beyond published hours of operation will be turned over to building security at the end of each day.

MEETING OFFICES. The following ACS offices will be located in the Moscone Center:

Attendee Registration: North Lobby

Career Fair: Halls B & C

Exhibitor Registration: South Lobby

Exposition: Halls B & C

Finance Office: Room 110

Host Local Section Center: Lower North Lobby

Member Services: North Lobby

Press Center: South Lobby

Shuttle Desk: Outside West Lobby

The following offices are located at the identified properties:

THANK YOU

The society thanks the many volunteers of the ACS California and Santa Clara Valley Sections who are contributing to the 253rd ACS National Meeting & Exposition as division officers or program chairs, symposium organizers, session or award presiders, oral and poster presenters, short course or workshop instructors, career consultants, and society governance members.

Operations Offices: Grand Hyatt San Francisco, Hilton San Francisco Union Square, Hotel Nikko San Francisco, InterContinental San Francisco, Palace Hotel, Parc 55 San Francisco, Park Central San Francisco, San Francisco Marriott Marquis, San Francisco Marriott Union Square, Sir Francis Drake Hotel, W San Francisco, Moscone Center.

Governance Office: San Francisco Union Square, Union Square 22

Society Programs: San Francisco Union Square, Nob Hill 2/3

MOTHERS ROOM. For your convenience and privacy, ACS will provide a room for nursing mothers at the Moscone Center. Please see the ACS Operations Office, South Lobby, for access to the room.

SMOKING. ACS policy prohibits smoking in all rooms during ACS functions at the convention center and official hotels. Additionally, the convention center and many of the official hotels are designated as smoke-free environments at all times.

GOVERNANCE & BUSINESS MEETINGS

MANY MEMBERS PARTICIPATE in meetings concerning the business of the Society, technical divisions, and governance committees in conjunction with the meeting. On the following pages, you will find a listing of the open meetings scheduled for San Francisco. ACS encourages its members to get active in governance at all levels in order to contribute their vision to the direction of the Society. You can share ideas and insights into the Society and the chemical profession, network with peers, and catch up with friends through these volunteer connections. With nearly thirty national governance committees and leadership opportunities in technical divisions and local sections to choose from, there are many opportunities for members to become actively involved in ACS at the national level. If you are an ACS member interested in volunteering for a governance committee, contact the Office of the Secretary by email at secretary@acs.org or by phone 202-872-4461. Someone will put you in contact with the ACS Committee on Committees to discuss your desire to volunteer for a committee assignment. If you wish to volunteer with a specific technical division or local section, contact the officers listed at www.acs.org to explore your specific interests.

ACS COUNCIL

The ACS Council meeting will begin at 8:00 AM, Wednesday, April 5, at the Hilton San Francisco Union Square. The meeting will be preceded by a continental breakfast for councilors beginning at 7:00 AM. Councilors are asked to check in beginning at 7:00 AM and proceed to the breakfast area, keeping in mind that the meeting starts promptly at 8:00 AM. Space will be available for ACS members and nonmembers to observe the council in action. We hope that many will take advantage of this opportunity to learn firsthand of the society's operation. Alternate councilors and division and local section officers are particularly urged to attend.

Golden Gate Bridge. SHUTTERSTOCK

GOVERNANCE MEETINGS

BOARD & COUNCIL MEETINGS

ACS Board of Directors. The ACS Board of Directors meeting, open to members who wish to participate, will be held in the Moscone Convention Center from noon to 1:00 PM on Sunday, April 2.

ACS Council. The ACS Council meeting will begin at 8:00 AM, Wednesday, April 5, at the Hilton San Francisco Union Square Hotel. The meeting will be preceded by a continental breakfast for councilors beginning at 7:00 AM. Councilors are asked to check in beginning at 7:00 AM and proceed to the breakfast area, keeping in mind that the meeting starts promptly at 8:00 AM. Space will be available for ACS members and nonmembers to observe the council in action. We hope that many will take advantage of this opportunity to learn firsthand of the society's operation. Alternate councilors and division and local section officers are particularly urged to attend.

COUNCILOR CAUCUS MEETINGS

District I Councilor Caucus
Sunday, April 2, 6:00 to 7:00 PM
Hilton San Francisco Union Square
Union Square 1/2

District II Councilor Caucus
Sunday, April 2, 6:00 to 7:00 PM
Hilton San Francisco Union Square
Union Square 3/4

District III Councilor Caucus
Sunday, April 2, 6:00 to 7:00 PM
Hilton San Francisco Union Square
Union Square 5/6

District IV Councilor Caucus
Sunday, April 2, 6:00 to 7:00 PM
Hilton San Francisco Union Square
Union Square 15/16

District V Councilor Caucus
Sunday, April 2, 6:00 to 7:00 PM
Hilton San Francisco Union Square
Union Square 17/18

District VI Councilor Caucus
Sunday, April 2, 6:00 to 7:00 PM
Hilton San Francisco Union Square
Union Square 19/20

Division Officers/Councilors Caucus
Tuesday, April 4, 4:00 to 6:00 PM
Moscone Convention Center
Room 132

COMMITTEE AGENDA

THE COMMITTEE ON COMMITTEES has clarified three types of committee meetings:

Open. May be attended by any ACS member. At these sessions, members are encouraged to voice concerns, issue compliments, offer suggestions, express interest in, or raise questions about matters over which the committee has purview. The assumption is that participation is welcomed and will be orderly and courteous. Only committee members can vote.

Executive. Attendance and participation are limited to officially appointed/ elected committee members, associates, advisers, consultants, staff liaisons, and the appointed Committee on Committees liaison. Liaisons from other groups and ex officio and elected councilors may attend; participation by these groups would be at the invitation of the chair. Only committee members can vote.

Closed. The committee chair must declare any executive session closed when confidential or sensitive personnel, financial, or legal matters of the society are discussed. At that point, only officially appointed/elected committee members, associates, consultants, staff liaisons, and the appointed Committee on Committees liaison shall remain in the session. Others may stay in the session at the discretion of the chair. Once these discussions have been completed, the committee should return to executive mode. During the open and executive committee meetings, ACS members are given a chance to express their views on issues under consideration before these issues are acted on by the board or the council, or to bring up other subjects that deserve attention.

Members are urged to examine the agenda and make known any opinions or ideas they may have. If you cannot attend the particular sessions involved, write to the officers listed or ask someone attending the session to speak on your behalf. For further information, contact the officers listed.

COUNCIL POLICY COMMITTEE

The Council Policy Committee will open the floor during its meeting at 11:30 AM on Tuesday, April 4, to councilors who would like to raise issues of concern that affect them and/or their local sections or divisions. For further information, contact

GOVERNANCE & BUSINESS MEETINGS

For the complete list of committee meetings and agendas, please consult www.acs.org/sanfran2017 or the on-site program for the meeting.

Budget & Finance

Joseph A. Heppert, chair; b_ffeedback@acs.org

Open Meeting
Saturday, April 1, 8:00 to 10:30 AM
Hilton San Francisco Union Square,
Imperial Ballroom B

1. *Report of the Chair*
2. *Report of the Treasurer & CFO:*
   a. *Budgetary Performance Report for the Year Ended December 31, 2016*
3. *Reports from the Subcommittees:*
   a. *Financial Impact of Constitution & Bylaw Changes*
   b. *Communications*
   c. *Program Funding Requests*
   d. *Program Review*

Chemical Safety

Elizabeth M. Howson, chair; safety@acs.org

Open Executive Session
Monday, April 3, 8:30 to 11:30 AM
Hilton San Francisco Union Square,
Continental Ballroom 6

1. *Welcome*
2. *Minutes of August 22 Meeting*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees and Task Forces:*
5. *New and Old Business*

Chemistry & Public Affairs

Raymond E. Forslund, chair; reforslund@me.com

Open Meeting
Saturday, April 1, 3:00 to 4:30 PM
Hilton San Francisco Union Square, Continental Ballroom 4

1. *Reports from the Subcommittees:*
   a. *Member Advocacy*
   b. *Public Policy*
   c. *Fellowships*
2. *Committee Liaison Reports*
3. *Public Comment*
4. *Closing Comments*

Chemists with Disabilities

John J. Johnston, chair; USDA-FSIS, 2150 Centre Ave, Fort Collins, CO 80526-8116

Open Executive Session
Sunday, April 2, 8:30 AM to 4:30 PM
Hilton San Francisco Union Square, Continental 1/2

1. *Welcome*
2. *Chair Report*
   a. *Update of CWD Activities/Events, and Collaborative Opportunities*
   b. *Diversity & Inclusion Advisory Group Report*
   c. *Minutes from (Philadelphia 2016)*
3. *Strategic Planning Group Updates*
4. *Discussion on Gender Neutral/Gender Inclusive Pronouns*
5. *Discussion on Awards and Travel Grants*
6. *CWD Poster Project*
7. *ACS Fellows Program*
8. *CWD Visibility (Social Media)*
9. *Other Action Items from Philadelphia Meeting*
10. *Staff Report*
11. *Future Event and Programming Planning*
12. *Subcommittee Progress Reports*
13. *Reports of Liaisons to/from other committees*
14. *Ongoing Business*
15. *New Business*

Committees

Wayne E. Jones Jr., chair; Department of Chemistry, Binghamton University, SUNY, 4400 Vestal Pkwy. East, Binghamton, NY 13902-6000

Open Meeting
Monday, April 3, 1:30 to 2:15 PM
Hilton San Francisco Union Square, Continental 8/9

1. *Welcome*
2. *Minutes of August 22–24, 2016*
3. *Reports of chair/staff liaison*
4. *Report of Subcommittees and Task Forces:*
   a. *Diversity*
   b. *Leadership Development*
   c. *Society Committee Bylaws*
5. *Topics from floor*

Community Activities

Michael B. McGinnis, chair; dean, College of Science & Mathematics, Norwich University, 158 Harmon Dr., Northfield, VT 05663

Executive Session
Sunday, April 2, 10:00 AM to noon
Hilton San Francisco Union Square, Grand Ballroom A

1. *Chair's welcome and comments*
2. *Reports from liaisons*
3. *Reports from subcommittees on:*
   a. *Program Development and Promotion*
   b. *Tools & Training*
   c. *Volunteer Engagement and Recognition*
4. *New business*

CCA/LSAC Joint Open Meeting
Tuesday, April 4, 2:00 to 3:30 PM
Hilton San Francisco Union Square

1. *Report from the LSAC and CCA Executive Sessions*
2. *Interactive session: questions, answers and best practices*

Constitution & Bylaws

James C. Carver, chair, the Carver Law Firm, 451 Florida St., Ste. 750, Baton Rouge, LA; bylaws@acs.org

Open Meeting
Sunday, April 2, 1:30 to 1:45 PM
Hilton San Francisco Union Square, Golden Gate 8

Open forum to discuss bylaws, petitions, and other issues that may arise

Executive Session
Sunday, April 2, 9:30 to 11:15 AM and 1:45 to 4:30 PM
Hilton San Francisco Union Square, Golden Gate 8

1. *Petition on International Chemical Sciences Chapters*
2. *Petitions, procedures, IAC Charter bylaws, and other items for action by Council*
3. *Bylaw Templates, questions document, and model bylaws*
4. *Bulletin 5 review and discussion*
5. *Reports from liaisons*
6. *Status of unit bylaws*
7. *Other business*

Corporation Associates

Diane Grob Schmidt, chair; d_schmidt@acs.org

Open Meeting
Monday, April 3, 8:00 AM to noon
Hilton San Francisco Union Square, Continental Ballroom 4

1. *Welcome*
2. *Approval of Minutes from San Diego, March 14, 2016*
3. *Chair's Report*
4. *Reports from Subcommittee Chairs*
   a. *Strategic Investment and Awards*
   b. *Public Policy*
   c. *CA Relations*
   d. *CA Member Value*
5. *Staff liaison report*
6. *New Business*

Council Policy

Mary K. Carroll, vice chair; cpc@acs.org

Open Executive Session
Tuesday, April 4, 9:30 AM to noon
Hilton San Francisco Union Square, Imperial Ballroom A

1. *Committee and Officer Reports*
2. *Report of CPC vice chair*
3. *Reports of Subcommittees on:*
   a. *Petitions, Constitution & Bylaws*
   b. *Long-Range Planning*
   c. *Nominations*
4. *Schedule of business sessions, fall 2017*
5. *Review of Council agenda*
6. *Open forum*
7. *Old and new business*

Divisional Activities

Rodney M. Bennett, chair; rodbennettdac@gmail.com

Open Meeting
Sunday, April 2, 8:00 AM to noon
Hilton San Francisco Union Square, Yosemite B

1. *Welcome*
2. *Review San Francisco agenda*
3. *Minutes from 252nd ACS National Meeting in Philadelphia, PA*
4. *Allocation formula*
5. *DAC Chair Report*
6. *Subcommittee Reports*

Economic & Professional Affairs

Rick Ewing, chair; ewingwre@comcast.net

Executive Session
Saturday, April 1, 8:00 to 10:30 AM
Hotel Nikko San Francisco, Nikko Ballroom I/II

1. *Opening Remarks*
2. *Invited Guest Reports*
3. *Staff Reports*

Open Meeting
Saturday, April 1, 10:30 AM to noon
Hotel Nikko San Francisco, Nikko Ballroom I/II

1. *Subcommittee Reports*
   a. *Public Policy*
   b. *Events, Volunteers and Employment Services*
   c. *Marketing and Research*
   d. *Standards and Ethics*
2. *Reports from Liaisons to and from CEPA*
3. *Ongoing Business/New Business*

Education

Diane Krone, chair; kroned@alumni.stevens.edu

Open Meeting
Monday, April 3, 3:00 to 4:00 PM
Hilton San Francisco Union Square, Golden Gate 8

Review of meeting, as below, plus items from the floor.

Executive Session
Friday, March 31, 1:00 to 5:30 PM
Hotel Nikko San Francisco, Nikko Ballroom I/II

1. *K-12 science topics, including ChemCom, ChemMatters, the American Association of Chemistry Teachers, High School Chemistry Clubs, Chemistry Olympiad, ACS-Hach programs, and teacher professional development*
2. *College/university topics, including undergraduate programs, graduate and postdoctoral education, ChemIDP, Chemistry in Context, and faculty development*

Items 1–2 open to all Councilors with prior approval of the Chair

Environmental Improvement

Anthony "Tony" Noce, chair; cei@acs.org

Breakfast/Open Meeting
Monday, April 3, 7:45 to 9:00 AM
San Francisco Marriott Marquis, Nob Hill D

1. *Review of the Saturday-Sunday CEI Executive Session*
2. *Overview of CEI activities in San Francisco*
3. *Planning of CEI activities in Washington*
4. *Preview of 2017 policy statement development (sustainability, scientific integrity)*
5. *Open discussion period*

Ethics

Keith Vitense, chair; Cameron University, Physical Science Department, 2800 West Gore Blvd., Lawton, OK 73505-6320

Open Executive Session
Sunday, April 2, 9:00 AM to 4:30 PM
Hilton San Francisco Union Square, Golden Gate 7

1. *Welcome & Introductions*
2. *Approval of Minutes from Philadelphia Meeting*
3. *Review of Committee on Ethics Charge*
4. *Chair/Staff Liaison Reports*
5. *Liaison Reports*
6. *Subcommittee Progress Reports*
7. *Committee Discussion*
8. *Subcommittee Working Sessions*
9. *Programming*
10. *Old Business/New Business/Action Items*
11. *Adjourn*

International Activities

Ellene Tratras Contis, chair; c/o ACS Office of International Activities, 1155 16th St., N.W., Washington, D.C. 20036

Open Meeting
Saturday, April 1, 1:00 to 3:00 PM
Hilton San Francisco Union Square, Continental 1/2

1. *Welcome*
2. *Minutes of August 20, 2016 IAC Meeting in Philadelphia*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees:*
   a. *Subcommittee on Africa and the Americas*
   b. *Subcommittee on Europe and the Middle East*
   c. *Subcommittee on Asia/Pacific Rim*
5. *New Business*

Local Section Activities

Jason E. Ritchie, chair, University of Mississippi Department of Chemistry & Biochemistry; 222 Coulter Hall, University, MS 38677; jritchie@olemiss.edu

LSAC/CCA Joint Open Meeting
Tuesday, April 4, 2:00 to 3:30 PM
Hilton San Francisco Union Square, Continental 1–3

1. *Report from the LSAC and CCA Executive Sessions*
2. *Interactive session: questions, answers and best practices*

Open Executive Session
Sunday, April 2, 8:00 AM to noon
Hilton San Francisco Union Square

1. *Report of chair, subcommittee chairs, staff liaison*
2. *Review of petitions for Council consideration*
3. *Reports of committee liaisons*

Meetings & Expositions

Kevin J. Edgar, chair; M&E@acs.org

Open Executive Session
Sunday, April 2, 7:30 to 10:00 AM
Moscone Center, Room 134

1. *Welcome*
2. *Minutes from Philadelphia*
3. *Chair's Report*
4. *Subcommittee Reports*
   a. *Expositions*
   b. *Technical Programming*
   c. *Regional Meetings*

Closed Executive Session
Sunday, April 2, 10:00 AM to noon
Moscone Center, Room 134

1. *Operations Subcommittee & Financial Report*
2. *Staff Liaison Report*
3. *New Business*

Membership Affairs

Margaret J. Schooler, chair; 5 Alexander Court, Hockessin, DE 19707-9797; margaret.j.schooler@axaltacs.com

Open Executive Session
Sunday, April 2, 3:00 to 4:00 PM
Hilton San Francisco Union Square, Grand Ballroom B

1. *Welcome*
2. *Minutes of August 21, 2016*
3. *Reports of Chair/Staff Liaison*
4. *Committee Strategic Planning Conference*
5. *Reports of Subcommittees*
   a. *Categories & Dues*
   b. *Retention, Benefits & Services*
   c. *Recruitment & Admissions*
6. *International Chapter Recruiting Trial Extension*
7. *Board "Collaborative for Re-Imagining a Diverse ACS Membership"*
8. *Topics from floor*

Minority Affairs

Madeleine Jacobs, chair; madeleine.s.jacobs@gmail.com

Closed Executive Session
Sunday, April 2, 8:00 AM to 12:30 PM
Hilton San Francisco Union Square, Continental Ballroom 4

1. *Opening Remarks*
2. *Staff Report*
3. *Fall Meeting Minutes*
4. *Subcommittee Meetings*

Open Meeting
Sunday, April 2, 12:30 to 2:00 PM
Hilton San Francisco Union Square, Continental Ballroom 4

1. *Subcommittee Reports*
2. *Old Business*
3. *New Business*

Nomenclature, Terminology & Symbols

Michael D. Mosher, chair; University of Northern Colorado; michael.mosher@unco.edu

Open Meeting
Monday, April 3, 2:00 to 5:00 PM
Hilton San Francisco Union Square, Continental Ballroom 5

1. *Review minutes from 2016 Fall National Meeting*
2. *Chair/Staff Liaison reports*
3. *Subcommittee Reports*
   a. *Communication/Outreach*
   b. *Education*
   c. *Liaison*
   d. *Long Range Planning*
4. *IUPAC Reports*
5. *New Business*

Nominations & Elections

Les W. McQuire, chair; nomelect@acs.org

Open Executive Session
Monday, April 3, 11:30 AM to noon
Hilton San Francisco Union Square, Imperial Ballroom A

1. *Report of the Executive Session*
2. *Vote 2020 Task Force*
3. *Topics from floor*

Patents & Related Matters

Sadiq Shah, chair; sadiq@utpa.edu

Open Meeting
Saturday, April 1, 9:00 AM to 5:00 PM
Hilton San Francisco Union Square, Imperial Ballroom A

1. *Legislation & Regulation Subcommittee.*
2. *Education and Outreach Subcommittee.*
3. *Awards Subcommittee.*
4. *Executive Session*

Professional Training

Thomas J. Wenzel, chair; Department of Chemistry, Bates College; cpt@acs.org

Open Meeting
Sunday, April 2, 4:00 to 5:00 PM
Hotel Nikko San Francisco, Peninsula

1. *Macromolecular curriculum requirement*
2. *Value of ACS approval of chemistry programs*
3. *Value of ACS certification to students*
4. *Applying for ACS approval*
5. *CPT survey of online instruction and virtual labs*
6. *CPT symposium on undergraduate research*
7. *Topics from floor*

Project SEED

Anna G. Cavinato, chair; department of chemistry, Eastern Oregon University, One University Blvd., LaGrande, OR 97850-2807

Open Meeting
Sunday, April 2, 9:30 to 10:30 AM
Hilton San Francisco Union Square, Union Square 15/16

1. *Report from executive session*
2. *Topics from the floor*

Closed Executive Session
Saturday, April 1, 10:30 AM to 5:00 PM
Hilton San Francisco Union Square, Union Square 17/18

1. *Subcommittee meetings 10:30 AM to 12:00 noon*
2. *Minutes of August 20, 2016*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees:*
5. *Old and new business*

Publications

Nicole S. Sampson, chair; Department of Chemistry, Stony Brook University, Stony Brook, NY 11794-3400

Open Meeting
Friday, March 31, 4:30 to 5:00 PM
Hotel Nikko San Francisco, Golden Gate

1. *Updates from ACS Publications Division*
2. *Open Discussion*

Science

Mark C. Cesa, chair; markcesa@comcast.net

Open Meeting
Saturday, April 1, 8:30 AM to 4:30 PM
Hilton San Francisco Union Square, Continental 3

1. *Welcome*
2. *Approval of Minutes*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees:*
   a. *Science and Technology,*
   b. *Awards,*
   c. *Public Policy and Communication*
5. *Subcommittee Breakouts*
6. *Subcommittee Reports from Breakouts*

Senior Chemists

Thomas R. Beattie, chair; silvercircle@acs.org

Open Executive Session
Monday, April 3, 8:00 AM to 1:00 PM
Hilton San Francisco Union Square, Yosemite B

1. *Welcome and Introductions*
2. *Minutes from November 2016 & February 2017 Meetings*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees and Task Forces:*
   a. *Newsletter of Senior Chemists*
   b. *Programming for Senior Chemists*
   c. *Consulting and Mentoring*
   d. *SCC Group on the ACS Network*
   e. *ACS Local Section Subcommittee*
   f. *Community Education Subcommittee*
   g. *ChemLuminary Award Nominations 2017*
   h. *ACS Fellows Nomination Subcommittee*
5. *Senior Chemists Breakfast in San Francisco*
6. *Open Discussion/General Information*

Technician Affairs

Kara M. Allen, chair; cta@acs.org

Closed Executive Session
Sunday, April 2, 8:00 AM to 12:30 PM
Hilton San Francisco Union Square, Continental Ballroom 6

Open Executive Session
Sunday, April 2, 12:30 to 1:00 PM
Hilton San Francisco Union Square, Continental Ballroom 6

1. *Welcome and Introductions*
2. *Review of Philadelphia Minutes, August 21, 2016*
3. *Reports of Chair/Staff Liaison*
4. *Report of Subcommittees and Task Forces:*
   a. *Communications Subcommittee*
   b. *Awards & Recognition Subcommittee*
   c. *Professional Development Subcommittee*
5. *Topics from floor/Meeting feedback/Wrap-up*
6. *Open Executive Session*

Women Chemists

Laura Sremaniak, chair; wcc@acs.org

Closed Executive Session
Saturday, April 1, 8:00 AM to 5:00 PM
Hilton San Francisco Union Square, Continental Ballroom 6

1. *Welcome*
2. *Review of Fall Action Items & Minutes*
3. *Reports of Chair/Staff Liaison*
4. *Subcommittee Meetings*
5. *Reports of Subcommittees and Task Forces:*
   a. *Awards & Recognition*
   b. *Communications & Technology*
   c. *Professional Development*
   d. *Programs & Events*
6. *New Business*

Younger Chemists

Natalie A. LaFranzo, chair; nlafranzo@gmail.com

Open Meeting
Sunday, April 2, 8:00 AM to noon
Hilton San Francisco Union Square, Continental Ballroom 5

1. *Welcome*
2. *Staff Report*
3. *Subcommittee Reports*
   a. *Communications*
   b. *Governance Interface and Outreach*
   c. *Membership Engagement*
4. *Liaison Reports*
5. *Petitions (CLOSED)*
6. *New Business*
7. *Visitors*
8. *Adjourn*

Executive Session
Sunday, April 2, noon to 1:00 PM
Hilton San Francisco Union Square, Continental Ballroom 5
Closed

DIVISION MEETINGS & SOCIAL EVENTS

Division of Agricultural & Food Chemmistry — AGFD

AGFD Poster Session Reception	Sunday, April 2	5:00 PM - 7:00 PM	West Hall, Moscone Convention Center
AGFD Future Program Meeting	Monday, April 3	12:00 PM - 1:00 PM	Yoskemite A, Hilton San Francisco Union Square
AGFD Executive Committee Meeting (CLOSED)	Monday, April 3	5:00 PM - 8:00 PM	Yoskemite A, Hilton San Francisco Union Square
AGFD Business Meeting	Tuesday, April 4	12:00 PM - 1:00 PM	Yoskemite A, Hilton San Francisco Union Square

Division of Analytic Chemistry — ANYL

ANYL Division Reception	Tuesday, April 4	5:00 PM - 7:30 PM	Golden Gate 2, Hilton San Francisco Union Square
ANYL Chemical Forensics International Technical Working Group Workshop	Wednesday, April 5	8:30 AM - 5:00 PM	Continental 4, Hilton San Francisco Union Square
ANYL Poster Session	Sunday, April 2	7:00 AM - 9:00 PM	West Hall, Moscone Convention Center

Division of Biochemical Technology — BIOT

Registration Table	Sunday, April 2	7:00 AM - 9:00 PM	SoMa, InterContinental San Francisco
Lunch Seminar	Sunday, April 2	12:30 PM - 2:00 PM	Intercontinental A, InterContinental San Francisco
Registration Table	Monday, April 3	7:00 AM - 9:00 PM	SoMa, InterContinental San Francisco
Lunch Seminar	Monday, April 3	12:30 PM - 2:00 PM	Intercontinental A, InterContinental San Francisco
Executive Committee Meeting (CLOSED)	Monday, April 3	7:00 PM - 10:00 PM	Marina, InterContinenta San Francisco
Registration Table	Tuesday, April 4	7:00 AM - 9:00 PM	SoMa, InterContinental San Francisco
Lunch Seminar	Tuesday, April 4	12:30 PM - 2:00 PM	Intercontinental A, InterContinental San Francisco
BIOT Poster Session Social	Tuesday, April 4	6:00 PM - 8:00 PM	West Hall, Moscone Convention Center
Registration Table	Wednesday, April 5	7:00 AM - 9:00 PM	SoMa, InterContinental San Francisco
Lunch Seminar	Wednesday, April 5	12:30 PM - 2:00 PM	Intercontinental A, InterContinental San Francisco
Program Chair Meeting (CLOSED)	Wednesday, April 5	12:30 PM - 2:00 PM	Russian Hill, InterContinental San Francisco
Future Programming Meeting	Wednesday, April 5	12:30 PM - 2:00 PM	Intercontinenal B, InterContinental San Francisco
Registration Table	Thursday, April 6	7:00 AM - 9:00 PM	SoMa, InterContinental San Francisco

Division of Biological Chemistry — BIOL

BIOL Poster Session/Social	Sunday, April 2	7:00 PM - 9:00 PM	West Hall, Moscone Convention Center
BIOL Poster Session/Social	Tuesday, April 4	7:00 PM - 9:00 PM	West Hall, Moscone Convention Center

Division of Business Development & Management — BMGT

Governance Meeting	Sunday, April 2	12:00 PM - 1:00 PM	Carmel I, Hotel Nikko San Francisco

Division of Catalysis & Surface Science — CATL

CATL Business Meeting	Monday, April 3	5:30 PM - 7:30 PM	Market Street, Parc 55 San Francisco

Division of Cellulose & Renewable Materials — CELL

Executive Committee Meeting (CLOSED)	Saturday, April, 1	4:00 PM - 7:30 PM	Room 262, Moscone Convention Center
Awards Banquet (TICKETED EVENT))	Tuesday, April 4	6:30 PM - 10:00 PM	Chart House @ Pier 39
Governance Meeting	Wednesday, April 5	5:30 PM - 7:30 PM	Room 274, Moscone Convention Center
Technical Program Meeting	Wednesday, April 5	7:30 PM - 8:00 PM	Room 274, Moscone Convention Center

Division of Chemistry & Law — CHAL

Drug & Power Luncheon (TICKETED EVENT)	Monday, April 3	12:00 PM - 1:30 PM	Mourad, 140 New Montgomery Street
CHAL Reception	Monday, April 3	6:00 PM - 8:00 PM	Jillian's, 175 Fourth Street

Division of Chemical Health & Safety — CHAS

Laboratory Waste Management Workshop CANCELLED	Friday, March 31	8:00 AM - 5:00 PM	Room 120, Moscone Convention Center
The Laboratory Safety Workshop	Friday, March 31	8:00 AM - 5:00 PM	Room 121, Moscone Convention Center
Cannabis Extraction Analysis Workshop CANCELLED	Saturday, April 1	8:00 AM - 5:00 PM	Room 120, Moscone Convention Center
How to be an Effective Chemical Hygiene Officer	Saturday, April 1	8:00 AM - 5:00 PM	Room 121, Moscone Convention Center
Reactive Chemical Management for Laboratories & Pilot Plants	Saturday, April 1	8:00 AM - 5:00 PM	Room 125, Moscone Convention Center
Using ACS Resources to Teach Lab Safety CANCELLED	Saturday, April 1	8:00 AM - 5:00 PM	Room 124, Moscone Convention Center
Executive Committee Meeting	Sunday, April 2	8:00 AM - 12:00 PM	Franciscan I, Park Central San Francisco
Cannabis Subdivision Lunch (CLOSED)	Monday, April 3	11:45 AM - 1:15 PM	Concordia, Parck Central San Francisco

Division of Chemical Education — CHED

CHED Meeting - (CLOSED)	Friday, March 31	2:00 PM - 6:00 PM	Sierra A, San Francisco Marriott Marquis
Exams Institute Board of Trustees	Saturday, April 1	7:30 AM - 12:00 PM	Sierra A, San Francisco Marriott Marquis
Board of Publication	Saturday, April 1	7:30 AM - 12:00 PM	Sierra B, San Francisco Marriott Marquis
Biennial Conference on Chemical Education Meeting	Sunday, April 2	8:00 AM - 9:30 AM	Golden Gate Ballroom C3, San Francisco Marriott Marquis
GC18F Exams (CLOSED)	Saturday, April 1	8:00 AM - 5:00 PM	Sierra J, San Francisco Marriott Marquis
PH19 Exams (CLOSED)	Saturday, April 1	8:00 AM - 5:00 PM	Sierra H, San Francisco Marriott Marquis
GC18 Exams (CLOSED)	Saturday, April 1	8:00 AM - 5:00 PM	Sierra F, San Francisco Marriott Marquis
GC17PQ Exams (CLOSED)	Saturday, April 1	8:00 AM - 5:00 PM	Sierra E, San Francisco Marriott Marquis
Program Committee Meeting	Saturday, April 1	10:30 AM - 12:30 PM	Sierra C, San Francisco Marriott Marquis
Executive Committee Meeting	Saturday, April 1	1:00 PM - 5:30 PM	Golden Gate Ballroom B, San Francisco Marriott Marquis
International Activities Committee Meeting	Sunday, April 2	8:00 AM - 9:30 AM	Salon 1, San Francisco Marriott Marquis
OR17F Exams (CLOSED)	Sunday, April 2	8:00 AM - 5:00 PM	Sierra E, San Francisco Marriott Marquis
ACS Exams Workshop	Sunday, April 2	8:00 AM - 5:00 PM	Sierra F, San Francisco Marriott Marquis
Finance Committee Meeting (CLOSED)	Sunday, April 2	9:30 AM - 11:30 AM	Sierra H, San Francisco Marriott Marquis
Research Committee Meeting	Sunday, April 2	12:00 PM - 1:30 PM	Sierra H, San Francisco Marriott Marquis
High School/College Interface Luncheon (TICKETED EVENT)	Sunday, April 2	12:00 PM - 1:00 PM	Salon 7, San Francisco Marriott Marquis
Regional Meeting Committee	Sunday, April 2	12:00 PM - 2:00 PM	Sierra G, San Francisco Marriott Marquis

Long Range Planning Committee	Sunday, April 2	2:30 PM - 4:30 PM	Sierra G, San Francisco Marriott Marquis
CHED Safety Committee Meeting	Sunday, April 2	4:00 PM - 5:30 PM	Sierra H, San Francisco Marriott Marquis
Social Reception	Sunday, April 2	5:30 PM - 7:00 PM	Room 130, Moscone Convention Center
Younger Chemistry Education Scholars Committee Meeting	Monday, April 3	9:30 AM - 5:00 PM	Sierra H, San Francisco Marriott Marquis
New Member Committee Meeting	Monday, April 3	12:00 PM - 12:30 PM	Salon 1/2
Business Meeting	Monday, April 3	12:00 PM - 12:30 PM	Salon 1/2, San Francisco Marriott Marquis
ACS Exams Workshop (CLOSED)	Monday, April 3	12:30 PM - 1:00 PM	Sierra F, San Francisco Marriott Marquis

Division of Chemical Information — CINF

Awards Committee Meeting (CLOSED)	Saturday, April 1	12:30 PM - 2:30 PM	City Room, Pack Central San Francisco
Education Committee Meeting (CLOSED)	Saturday, April 1	12:30 PM - 2:30 PM	Franciscan II, Park Central San Francisco
Program/Executive Committee Meeting (CLOSED)	Saturday, April 1	12:30 PM - 6:00 PM	Franciscan I, Park Central San Francisco
Chemical Structure Association (CSAT) Meeting (CLOSED)	Sunday, April 2	12:00 PM - 2:00 PM	Franciscan II, Park Central San Francisco
Welcome Recption and Poster Session	Sunday, April 2	6:30 PM - 8:30 PM	Franciscan I & II, Park Central San Francisco
Luncheon (TICKETED EVENT)	Tuesday, April 4	12:00 PM - 1:30 PM	Franciscan I, Park Central San Francisco
Chemistry Research Data Interest Group (Research Data Alliance)	Wednesday, April 5	1:00 PM - 5:00 PM	Franciscan I, Park Central San Francisco

Division of Colloid & Surface Chemistry — COLL

Program & Executive Committee Meeting (CLOSED)	Saturday, April 1	4:00 PM - 7:00 PM	Room 133, Moscone Convention Center
Poster Session/Social Hour	Sunday, April 2	5:30 PM - 8:00 PM	Halls B/C, Moscone Convention Center
Division Luncheon (TICKETED)	Tuesday, April 4	12:00 PM - 1:30 PM	Great Room I, W San Francisco

Division of Computers in Chemistry — COMP

Executive Committee Meetings	Saturday, April 1	3:00 PM - 6:00 PM	Grand Ballroom B, InterContinental San Francisco
Poster Session	Tuesday, April 4	6:00 PM - 8:00 PM	West Hall, Mocone Convention Center

Division of Energy & Fuel — ENFL

Energy and Fuels Program Meeting	Sunday, April 2	12:00 PM - 2:00 PM	Redwood B, Grand Hyatt San Francisco
ENFL Executive Meeting	Sunday, April 2	4:00 PM - 7:00 PM	Sunset A/B, Grand Hyatt San Francisco
Energy and Fuel Business Meeting	Monday, April 3	5:00 PM - 7:00 PM	Grand Ballroom West, Grand Hyatt San Francisco
ENFL Dinner (TiCKETED)	Tuesday, April 4	6:30 PM - 9:00 PM	Le Colonial, 20 Cosmo Place

Division of Environmental Chemistry — ENVR

Program Planning Committee Meeting	Sunday, April 2	2:00 PM - 3:00 PM	Golden Gate Blrm C3, San Francisco Marriott Marquis
Long Range Planning Committee	Sunday, April 2	3:00 PM - 5:00 PM	Golden Gate Blrm C3, San Francisco Marriott Marquis
Executive Committee Meeting	Sunday, April 2	7:00 PM - 10:00 PM	Golden Gate Blrm C3, San Francisco Marriott Marquis
Division Reception (TICKETED EVENT)	Tuesday, April 4	6:00 PM - 8:00 PM	Thirsty Brewery Company, 661 Howard Street

Division of Geochemistry — GEOC

Executive Committee Meeting (CLOSED)	Sunday, April, 2	6:00 PM - 8:00 PM	Russian Hill, San Francisco Marriott Union Square
Social Event (CLOSED)	Tuesday, April 4	5:30 PM - 7:30 PM	Empire Ballroom, Sir Francis Drake

Division of History of Chemistry — HIST

Executive Committee Meeting (CLOSED)	Sunday, April 2	5:00 PM - 8:00 PM	Redwood B, Grand Hyatt San Francisco

Division of Industrial & Engineering Chemitry — I&EC

I&EC Subdivision, Steering & Programming Meeting (CLOSED)	Saturday, April 1	11:00 AM - 3:00 PM	Russian Hill, San Francisco Marriott Union Square

Division of Inorganic Chemistry — INOR

INOR Poster Session/Social	Sunday, April 2	5:30 PM - 7:30 PM	Hall D, Moscone Convention Center
INOR Poster Session/Social	Tuesday, April 4	5:30 PM - 7:30 PM	Hall D, Moscone Convention Center

Division of Medicinal Chemistry — MEDI

Executive Committee Meeting (CLOSED)	Sunday, April 2	8:30 AM - 1:00 PM	Room 133, Moscone Convention Center
Business Meeting (CLOSED)	Sunday, April 2	5:30 PM -6:30 PM	Room 133, Moscone Convention Center
General Poster Session	Sunday, April 2	7:00 PM - 9:00 PM	West Hall, Moscone Convention Center
MEDI Long Range Planning Committee (CLOSED)	Monday, April 3	5:30 PM - 10:00 PM	Great Room 1, W San Francisco
MEDI & ORGN General Poster Session	Wednesday, April 5	7:00 PM - 11:00 PM	West Hall, Moscone Convention Center

Division of Nuclear Chemistry & Technology — NUCL

Executive Committee Meeting (CLOSED)	Sunday, April 2	5:00 PM - 7:00 PM	Esplanade Blrm 308, Moscone Convention Center
Business Meeting	Tuesday, April 4	5:00 PM - 6:00 PM	Room 134, Moscone Convention Center
NUCL Social Hour	Tuesday, April 4	6:00 PM - 8:00 PM	Room 130, Moscone Convention Center

Division of Organic Chemistry — ORGN

Executive Committee Meeting (CLOSED)	Sunday, April 2	1:00 PM - 6:00 PM	Room 134, Moscone Convention Center
ORGN Poster Session/Social	Sunday, April 2	5:30 PM - 7:30 PM	West Hall, Moscone Convention Center

Division of Physical Science — PHYS

Executive Committee Meeting (CLOSED)	Sunday, April 2	4:30 PM - 7:30 PM	Powell Room, Parc 55 San Francisco - A Hilton Hotel
Molssi Kick-Off Reception	Tuesday, April 4	5:30 PM - 7:30 PM	Bayview, Hotel Nikko San Francisco
Division Poster Session	Wednesday, April 5	6:00 PM - 8:00 PM	Hall D, Moscone Convention Center

Division of Polymeric Materials — PMSE

Membership Desk	Sunday, April, 2	8:00 AM - 5:00 PM	Esplanade Ballroom Foyer, Moscone Convention Center
Executive Committee Meeting (CLOSED)	Sunday, April 2	4:30 PM - 7:00 PM	Room 132, Moscone Convention Center
Membership Desk	Monday, April 3	8:00 AM - 5:00 PM	Esplanade Ballroom Foyer, Moscone Convention Center
Business Meeting and PMSE/POLY Coordination	Monday, April 3	5:00 PM - 6:00 PM	2nd Floor, Area 2, Moscone Center West
Membership Desk	Tuesday, April 4	8:00 AM - 5:00 PM	Esplanade Ballroom Foyer, Moscone Convention Center
PMSE/POLY Joint Poster Session/Social	Tuesday, April 4	6:00 PM - 8:00 PM	Hall A, Moscone Center
Membership Desk	Wednesday, April 5	8:00 AM - 5:00 PM	Esplanade Ballroom Foyer, Moscone Convention Center
Membership Desk	Thursday, April 6	8:00 AM - 5:00 PM	Esplanade Ballroom Foyer, Moscone Convention Center

Division of Polymer Chemistry — POLY

Membership Desk	Sunday, April 2	8:00 AM - 5:00 PM	Rooms 120-123 Foyer, Moscone Convention Center
Workshop Committee (CLOSED)	Sunday, April 2	11:00 AM - 12:00 PM	Room 132, Moscone Convention Center
Board Meeting	Sunday, April 2	12:00 PM - 2:00 PM	Room 132, Moscone Convention Center
International Committee Meeting (CLOSED)	Sunday, April 2	2:00 PM - 4:00 PM	2nd Floor, Area 1, Moscone Center West
Stategic & Long Range Planning Meeting (CLOSED)	Sunday, April 2	4:00 PM - 5:30 PM	2nd Floor, Area 1, Moscone Center West
Membership Desk	Monday, April 3	8:00 AM - 5:00 PM	Rooms 120-123 Foyer, Moscone Convention Center
Financial/Executive Planning Meeting (CLOSED)	Monday, April 3	12:00 PM - 2:00 PM	2nd Floor, Area 1, Moscone Center West
Industrial Advisory Board Meeting (CLOSED)	Tuesday, April 4	8:00 AM - 10:00 AM	Room 133, Moscone Convention Center
Membership Desk	Tuesday, April 4	8:00 AM - 5:00 PM	Rooms 120-123 Foyer, Moscone Convention Center
POLY/IPEC Meeting (CLOSED)	Tuesday, April 4	9:00 AM - 12:00 PM	2nd Floor, Area 1, Moscone Center West
Programming Committee Meeting	Tuesday, April 4	1:00PM - 2:00 PM	Room 2000, Moscone Convention Center West
Membership Committee Meeting (CLOSED	Tuesday, April 4	2:00 PM - 3:00 PM	2nd Floor, Area 1, Moscone Center West
PMSE/POLY Joint Poster Session/Social	Tuesday, April 4	6:00 PM - 8:00 PM	Hall A, Moscone Center
Membership Desk	Wednesday, April 5	8:00 AM - 5:00 PM	Rooms 120-123 Foyer, Moscone Convention Center
POLY/PMSE Award Lecture & Reception	Wednesday, April 5	5:30 PM - 8:00 PM	Room 134, Moscone Convention Center
Membership Desk	Thursday, April 6	8:00 AM - 5:00 PM	Rooms 120-123 Foyer, Moscone Convention Center

Division of Professional Relations — PROF

Executive Committee Meeting	Tuesday, April 4	3:00 PM - 5:00 PM	Nikko Ballroom II, Hotel Nikko San Francisco
Henry Hill & Lou Sacco Award Reception	Tuesday, April 4	5:00 PM - 7: 00 PM	Nikko Ballroom II, Hotel Nikko San Francisco

Division of Small Chemical Business — SCHB

Executive Committee	Sunday, April 2	8:00 AM - 11:30 AM	Monterey II, Hotel Nikko San Francisco

SOCIAL & EDUCATIONAL EVENTS

PRESIDENTIAL EVENTS

ACS President Allison Campbell welcomes attendees to the 253rd ACS National Meeting. The presidential and cosponsored event symposia will focus on areas of significant importance: the health of our planet, the safe practice of science, and strong technical programming.

The first symposium, "**LGBT Graduate & Postdoctoral Student Chemistry Research,"** is organized by the Division of Professional Relations. This two-day symposium on Sunday, April 2 and Monday, April 3 will consist of scientific talks by LGBT graduate and postdoctoral students and will conclude with a panel discussion on issues that affect LGBT students and postdocs. Later Sunday afternoon at 1:20 PM, the symposium "**Holy Grails in Chemistry**: **Celebrating the 50th Anniversary of Accounts of Chemical Research Journal"** will focus on a 1995 issue in the journal that sought to spotlight critical areas of chemistry and will assess the progress in these areas since then.

On Monday, April 3, from 8:30 AM to 4:30 PM, the symposium "**Science for a Sustainable Energy Future"** will highlight scientific advances for creating and storing sustainable, low-carbon energy. The symposium will focus on advances in energy storage in the morning session and chemical and biological approaches to energy conversion in the afternoon.

Thirteen **president-recommended** symposia focus on issues of safety, communicating science, highlighting up-and-coming graduate researchers, and celebrating diverse practitioners of chemistry. Details of these presidential events and other recommended symposia can be found at www.acs.org/sanfran2017.

ACS 2017 NATIONAL AWARD WINNERS

THE ACS NATIONAL AWARDS recognize individual and team accomplishments in diverse fields of the chemical sciences. Award recipients traditionally receive their national award in person during the ACS awards dinner and general meeting and deliver an award address on the scientific work that is being recognized to an appropriate division.

This year's event will be held on the evening of Tuesday, April 4, at the San Francisco Marriott Marquis, Yerba Buena Ballroom, Salons 8/9. Dinner begins at 7:30 PM, and the general meeting begins at 8:30 PM.

Tobin J. Marks will deliver the Priestley Medal Address at the general meeting. See Ticketed Events on page 38 for ticket information.

Several awards, such as the Arthur C. Cope Scholar Awards and the Arthur C. Cope Award, will be presented at the Arthur C. Cope Symposium in conjunction with the 254th ACS National Meeting in Washington, D.C. in August.

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry, sponsored by the ACS Exams Institute, **Marcy H. Towns,** Purdue University. Address to be presented before the Division of Chemical Education. April 3; San Francisco Marriott Marquis; Salons 1/2; 3:55 PM.

ACS Award for Affordable Green Chemistry, sponsored by Dow Chemical Co. and endowed by Rohm and Haas, **Peter J. Dunn,** Pfizer (retired). Address to be presented before the Division of Industrial & Engineering Chemistry. April 4; Grand Hyatt San Francisco; Fillmore C; 11:35 AM.

ACS Award for Computers in Chemical & Pharmaceutical Research, sponsored by the ACS Division of Computers in Chemistry, **Yvonne Connolly Martin,** Abbott Laboratories, AbbVie**.** Address to be presented before the Division of Computers in Chemistry. April 4; InterContinental San Francisco; Laurel Hill; 4:15 PM.

ACS Award for Creative Advances in Environmental Science & Technology, sponsored by the ACS Division of Environmental Chemistry and the ACS Publications journals Environmental Science & Technology and Environmental Science & Technology Letters, **Douglas R. Worsnop,** Aerodyne Research and University of Helsinki, Finland. Address to be presented before the Division of Environmental Chemistry. April 4; San Francisco Marriott Marquis; Salons 10/11; 4:15 PM.

ACS Award for Creative Invention, sponsored by ACS Corporation Associates, **Richard B. Silverman,** Northwestern University. Address to be presented before the Division of Medicinal Chemistry. April 4; Moscone Center; 3002/3004; 10:30 AM.

ACS Award for Creative Work in Fluorine Chemistry, sponsored by the ACS Division of Fluorine Chemistry, **Antonio Togni,** Swiss Federal Institute of Technology, (ETH) Zurich. Address to be presented before the Division of Fluorine Chemistry. April 3; Grand Hyatt San Francisco; Sequoia; 11:15 AM.

ACS Award for Creative Work in Synthetic Organic Chemistry, sponsored by MilliporeSigma, **Matthew S. Sigman,** University of Utah. Address to be presented before the Division of Organic Chemistry. April 4; Moscone Center; 3018/3022; 11:15 AM.

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry, sponsored by Strem Chemicals, **William B. Tolman,** University of Minnesota, Twin Cities. Address to be presented before the Division of Inorganic Chemistry. April 3; Moscone Center; Gateway Ballroom 103/104; 8:15 AM.

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences, sponsored by the Camille and Henry Dreyfus Foundation, **Saundra Yancy McGuire,** Louisiana State University. Address to be presented before the Division of Chemical Education. April 4; San Francisco Marriott Marquis; Salons 3/4; 10:35 AM.

ACS Award for Encouraging Women into Careers in the Chemical Sciences, sponsored by the Camille and Henry Dreyfus Foundation, **Judith M. Iriarte-Gross,** Middle Tennessee State University. Address to be presented before the ACS Women Chemists Committee and the Division of Chemical Education. April 4; Hotel Nikko San Francisco; Monterey II; 10:50 AM.

ACS Award for Research at an Undergraduate Institution, sponsored by Research Corporation for Science Advancement, **Maria R. Hepel,** SUNY at Potsdam. Address to be presented before the Division of Colloid and Surface Chemistry. April 4; Moscone Center; 2002; 3:45 PM.

ACS Award for Team Innovation, sponsored by ACS Corporation Associates, **Robert A. DeVries,** R DeVries Consulting, LLC; **Philip E. Garrou,** Microelectronic Consultants of North Carolina**; Carol E. Mohler** and **Theodore M. Stokich, Jr. (Ted),** Dow Chemical**; Eric Scott Moyer,** LORD Corporation. Address to be presented before the Division of Polymeric Materials: Science & Engineering. April 5; Moscone Center; Esplanade Ballroom 307; 3:40 PM.

ACS Award in Analytical Chemistry, sponsored by the Battelle Memorial Institute, **Donald Frederick Hunt,** University of Virginia. Address to be presented before the Division of Analytical Chemistry. April 3; Hilton San Francisco Union Square; Franciscan D; 4:00 PM.

ACS Award in Applied Polymer Science, sponsored by Eastman Chemical, **Zhenan Bao,** Stanford University. Address to be presented before the Division of Polymeric Materials: Science & Engineering. April 3; Moscone Center; Esplanade Ballroom 304; 4:30 PM.

ACS Award in Chromatography, sponsored by MilliporeSigma, **Robert T. Kennedy,** University of Michigan. Address to be presented before the Division of Analytical Chemistry. April 3; Hilton San Francisco Union Square; Franciscan D; 10:55 AM.

ACS Award in Colloid Chemistry, sponsored by Colgate-Palmolive Co., **Nicholas Alexander Kotov,** University of Michigan. Address to be presented before the Division of Colloid & Surface Chemistry. April 4; Moscone Center; 2002; 2:05 PM.

ACS Award in Industrial Chemistry, sponsored by the ACS Division of Industrial & Engineering Chemistry, **Jane Frommer,** IBM Research. Address to be presented before the Division of Industrial & Engineering Chemistry and the Division of Organic Chemistry. April 3; Grand Hyatt San Francisco; Fillmore C; 1:35 PM.

ACS Award in Inorganic Chemistry, sponsored by Aldrich Chemical Co., LLC, **Lawrence Que, Jr.,** University of Minnesota, Twin Cities. Address to be presented before the Division of Inorganic Chemistry. April 3; Moscone Center; Gateway Ballroom 103/104; 9:20 AM.

ACS Award in Organometallic Chemistry, sponsored by the Dow Chemical Co. Foundation, **Marcetta Y. Darensbourg,** Texas A&M University. Address to be presented before the Division of Inorganic Chemistry. April 3; Moscone Center; Gateway Ballroom 103/104; 10:10 AM.

ACS Award in Polymer Chemistry, sponsored by ExxonMobil Chemical, **Murugappan Muthukumar,** University of Massachusetts, Amherst. Address to be presented before the Division of Polymer Chemistry. April 5; Moscone Center; Esplanade Ballroom 310; 4:30 PM.

ACS Award in Pure Chemistry, sponsored by the Alpha Chi Sigma Fraternity and the Alpha Chi Sigma Educational Foundation, **Neal K. Devaraj,** University of California, San Diego. Address to be presented before the Division of Biological Chemistry. April 2; Moscone Center; 3014/3016; 4:30 PM.

ACS Award in Separations Science & Technology, sponsored by Waters Corp., **Rakesh Agrawal,** Purdue University. Address to be presented before the Industrial & Engineering Chemistry Separations Science & Technology Symposium at the fall ACS national meeting in Washington, D.C.

ACS Award in Surface Chemistry, sponsored by the ACS Division of Colloid & Surface Chemistry, **Cynthia M. Friend,** Harvard University. Address to be presented before the Division of Colloid & Surface Chemistry. April 4; Moscone Center; 2002; 2:55 PM.

ACS Award in the Chemistry of Materials, sponsored by DuPont, **Douglas A. Keszler,** Oregon State University. Address to be presented before the Division of Inorganic Chemistry. April 3; Moscone Center; Gateway Ballroom 103/104; 11:40 AM.

ACS Award in Theoretical Chemistry, sponsored by the ACS Division of Physical Chemistry, **Peter Pulay,** University of Arkansas. Address to be presented before the Division of Physical Chemistry. April 4; Parc 55 San Francisco; Embarcadero; 11:00 AM.

Award for Volunteer Service to the American Chemical Society, sponsored by ACS, **D. Richard Cobb,** Eastman Kodak Company (retired). Address to be presented before the ACS ChemLuminary Awards at the fall ACS national meeting in Washington, D.C.

Roger Adams Award in Organic Chemistry, sponsored by Organic Reactions, Inc. and Organic Syntheses, Inc., **Hisashi Yamamoto,** Chubu University, Japan. Address to be presented before the National Organic Chemistry Symposium in Davis, CA.

Alfred Bader Award in Bioinorganic or Bioorganic Chemistry, sponsored by the Alfred R. Bader Fund, **Kim D. Janda,** Scripps Research Institute. Address to be presented before the Division of Organic Chemistry at the fall ACS national meeting in Washington, D.C.

Earle B. Barnes Award for Leadership in Chemical Research Management, sponsored by the Dow Chemical Co. Foundation, **Laurie E. Locascio,** National Institute of Standards & Technology. Address to be presented before the Division of Analytical Chemistry at the fall ACS national meeting in Washington, D.C.

Ronald Breslow Award for Achievement in Biomimetic Chemistry, sponsored by the Ronald Breslow Award Endowment, **Benjamin G. Davis,** University of Oxford, England. Address to be presented before the Division of Biological Chemistry. April 2; Moscone Center; 131; 11:40 AM.

Herbert C. Brown Award for Creative Research in Synthetic Methods, sponsored by the Purdue Borane Research Fund and the Herbert C. Brown Award Endowment, **Bruce H. Lipshutz,** University of California, Santa Barbara. Address to be presented before the Division of Organic Chemistry. April 2; Moscone Center; 3018/3022; 4:00 PM.

James Bryant Conant Award in High School Chemistry Teaching, sponsored by the Journal of Chemical Education and ChemEd X, **Laura Elizabeth Slocum,** Heathwood Hall Episcopal School, South Carolina. Address to be presented before the Division of Chemical Education. April 2; San Francisco Marriott Marquis; Golden Gate C2/C3; 1:10 PM.

Arthur C. Cope Award, sponsored by the Arthur C. Cope Fund, **Carolyn R. Bertozzi,** Stanford University and Howard Hughes Medical Institute. Address to be presented before the Division of Organic Chemistry at the fall ACS national meeting in Washington, D.C.

Arthur C. Cope Scholar Awards, sponsored by the Arthur C. Cope Fund, **Alejandro L. Briseno,** University of Massachusetts, Amherst; **Sherry R. Chemler,** University of Buffalo, SUNY; **Guangbin Dong,** University of Texas at Austin and University of Chicago; **P. Andrew Evans,** Queen's University; **M.G. Finn,** Georgia Institute of Technology; **Paul J. Hergenrother,** University of Illinois, Urbana-Champaign; **Thomas R. Hoye,** University of Minnesota, Twin Cities; **Kathlyn A. Parker,** Stony Brook University, SUNY; **Mikiko Sodeoka,** RIKEN, Japan; **Christopher D. Vanderwal,** University of California, Irvine. Address to be presented before the Division of Organic Chemistry at the fall ACS national meeting in Washington, D.C.

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator sponsored by the Pfizer Endowment Fund, **Neil K. Garg,** University of California, Los Angeles. Address to be presented before the Division of Organic Chemistry. April 3; Moscone Center; 3018/3022; 11:00 AM.

F. Albert Cotton Award in Synthetic Inorganic Chemistry, sponsored by the F. Albert Cotton Endowment Fund, **Pingyun Feng,** University of California, Riverside. Address to be presented before the Division of Inorganic Chemistry. April 3; Moscone Center; Gateway Ballroom 103/104; 10:40 AM.

Peter Debye Award in Physical Chemistry, sponsored by DuPont, **Bruce J. Berne,** Columbia University. Address to be presented before the Division of Physical Chemistry. April 3; Parc 55 San Francisco; Embarcadero; 8:00 AM.

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry, sponsored by Waters Corp., **Vicki Hopper Wysocki,** Ohio State University. Address to be presented before the Division of Analytical Chemistry. April 4; Hilton San Francisco Union Square; Union Square 19/20; 1:35 PM.

Francis P. Garvan–John M. Olin Medal, sponsored by the Francis P. Garvan–John M. Olin Medal Endowment, **Barbara J. Finlayson-Pitts,** University of California, Irvine. Address to be presented before the Division of Physical Chemistry. April 5; Parc 55 San Francisco; Embarcadero; 8:05 AM.

James T. Grady–James H. Stack Award for Interpreting Chemistry for the Public, sponsored by ACS, **Thomas A. Hager,** University of Oregon. Address to be presented before the ACS Office of Public Affairs, Division of Chemical Education and the Division of the History of Chemistry at the fall ACS national meeting in Washington, D.C.

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator, sponsored by the Gray Award Endowment, **Nilay Hazari,** Yale University. Address to be presented before the Division of Inorganic Chemistry. April 3; Moscone Center; Gateway Ballroom 103/104; 8:50 AM.

Ernest Guenther Award in the Chemistry of Natural Products, sponsored by Givaudan, **Stephen F. Martin,** University of Texas at Austin. Address to be presented before the Division of Organic Chemistry. April 3; Moscone Center; 3018/3022; 3:45 PM.

Kathryn C. Hach Award for Entrepreneurial Success, sponsored by the Kathryn C. Hach Award Fund, **David R. Walt,** Tufts University. Address to be presented before the Division of Analytical Chemistry and the Division of Biochemical Technology. April 4; Hilton San Francisco Union Square; Union Square 19/20; 10:55 AM.

E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances, sponsored by Merck Research Laboratories, **Stanley T. Crooke,** Ionis Pharmaceuticals. Address to be presented before the Division of Medicinal Chemistry. April 4; Moscone Center; 3002/3004; 9:45 AM.

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids, sponsored by ExxonMobil Research & Engineering, **Salvatore Torquato,** Princeton University. Address to be presented before the Division of Physical Chemistry. April 3; Parc 55 San Francisco; Embarcadero; 4:30 PM.

E. V. Murphree Award in Industrial & Engineering Chemistry, sponsored by ExxonMobil Research & Engineering, **Eleftherios Terry Papoutsakis**, University of Delaware. Address to be presented before the Division of Biochemical Technology. April 5; InterContinental San Francisco; Grand Ballroom B/C; 11:30 AM.

Nakanishi Prize, sponsored by the Nakanishi Prize Endowment, **Martin Gruebele,** University of Illinois, Urbana-Champaign. Address to be presented before the Division of Physical Chemistry. April 3; Parc 55 San Francisco; Powell I/II; 9:00 AM.

Nobel Laureate Signature Award for Graduate Education in Chemistry, sponsored by Avantor Performance Materials, **Junqi Li (student)** and **Martin D. Burke (preceptor),** University of Illinois, Urbana-Champaign. Address to be presented before the Division of Organic Chemistry. April 5; Moscone Center; 3018/3022; 11:15 AM & 10:30 AM.

James Flack Norris Award in Physical Organic Chemistry, sponsored by the ACS Northeastern Section, **Robert A. Moss,** Rutgers University. Address to be presented before the Division of Organic Chemistry. April 4; Moscone Center; 3018/3022; 4:00 PM.

George A. Olah Award in Hydrocarbon or Petroleum Chemistry, sponsored by the George A. Olah Award Endowment, **Robert Howard Grubbs,** California Institute of Technology. Address to be presented before the Division of Organic Chemistry. April 2; Moscone Center; 3018/3022; 11:10 AM.

Charles Lathrop Parsons Award, sponsored by ACS, **John I. Brauman,** Stanford University. Address to be presented before the ACS Board of Directors. April 2; Moscone Center; 130; 1:30 PM.

George C. Pimentel Award in Chemical Education, sponsored by Cengage Learning and the ACS Division of Chem-

ical Education, **Thomas A. Holme,** Iowa State University. Address to be presented before the Division of Chemical Education. April 4; San Francisco Marriott Marquis; Salons 1/2; 3:55 PM.

Priestley Medal, sponsored by ACS, **Tobin J. Marks,** Northwestern University. Address to be presented at the ACS National Awards Banquet Ceremony & General Meeting of the Society at the spring national meeting in San Francisco.

Glenn T. Seaborg Award for Nuclear Chemistry, sponsored by the ACS Division of Nuclear Chemistry & Technology, **David L. Clark,** Los Alamos National Laboratory. Address to be presented before the Division of Nuclear Chemistry & Technology. April 2; Moscone Center; Esplanade Ballroom 302; 1:20 PM.

Gabor A. Somorjai Award for Creative Research in Catalysis, sponsored by the Gabor A. & Judith K. Somorjai Endowment Fund, **John E. Bercaw,** California Institute of Technology. Address to be presented before the Division of Inorganic Chemistry. April 3; Moscone Center; Gateway Ballroom 103/104; 11:10 AM.

E. Bright Wilson Award in Spectroscopy, sponsored by the ACS Division of Physical Chemistry, **David John Nesbitt,** Joint Institute for Lab Astrophysics/National Institute of Standards & Technology and University of Colorado. Address to be presented before the Division of Physical Chemistry. April 4; Parc 55 San Francisco; Embarcadero; 2:40 PM.

Ahmed Zewail Award in Ultrafast Science & Technology, sponsored by the Ahmed Zewail Endowment Fund established by the Newport Corp., **Stephen R. Leone,** University of California, Berkeley. Address to be presented before the Division of Physical Chemistry. April 2; Parc 55 San Francisco; Embarcadero; 9:40 AM.

National Fresenius Award, sponsored by Phi Lambda Upsilon, the National Chemistry Honor Society, **Neal K. Devaraj,** University of California, San Diego. Address to be presented before the Division of Organic Chemistry. April 2; Moscone Center; 3014/3016; 11:05 AM.

STUDENT & EDUCATOR ACTIVITIES

Education-focused programs and specialty activities are being held for undergraduate students, graduate students, high school teachers, and chemical professionals. Explore these opportunities in depth at www.acs.org/sanfran2017.

Undergraduate Program. A vibrant program designed especially for undergraduate students has been planned by the Society Committee on Education's Undergraduate Programs Advisory Board. This educational and career-oriented program includes technical symposia and workshops on essential skills for employment in chemistry and success in graduate school. Eminent scientist Dr. Carolyn Bertozzi of Stanford University will present, "What life and research share in common: Finding opportunity in failure."

Sunday, April 2

Undergraduate Hospitality Center, 8:00 AM to 5:00 PM, SF Marriott Marquis, Salon 7

Making the Most of your First National Meeting, 8:30 to 9:15 AM, SF Marriott Marquis, Salon 7

Undergraduate Research Oral Session, 8:30 AM to 5:00 PM, SF Marriott Marquis, Nob Hill C

Symposium: Frontiers in Nanoscience (cosponsored by POLY), 9:30 to 11:30 AM, SF Marriott Marquis, Golden Gate A

Chem Demo Exchange, 11:00 AM to 12:30 PM

Graduate School Reality Check, Step I: Getting In (cosponsored by YCC), 10:00 to 11:30 AM, SF Marriott Marquis, Golden Gate A

Graduate School Reality Check, Step II: You're In—Now What? (cosponsored by YCC), 11:30 AM to 12:45 PM

Networking Social with Graduate School Recruiters, 1:00 to 5:00 PM

Networking 101 (cosponsored by YCC and PROF), 1:30 to 3:00 PM, SF Marriott Marquis, Golden Gate A

Two-Year to Four-Year College Transfer Survival Guide (cosponsored by YCC), 2:30 to 3:30 PM, SF Marriott Marquis, Golden Gate B

SciBabe, Ten Rules to Surviving Fake News, 4:00 to 5:30 PM, SF Marriott Marquis, Golden Gate A

Student Awards Ceremony, 7:00 to 8:30 PM, Hilton Union Square, Grand Ballroom B

Undergraduate Social, 8:30 to 11:00 PM, Hilton Union Square, Continental Ballroom 1–6

Monday, April 3

Undergraduate Hospitality Center, 8:00 AM - 4:00 PM, SF Marriott Marquis, Salon 7

Undergraduate Research Oral Session, 8:30 AM to 5:00 PM, SF Marriott Marquis, Nob Hill C

Improving Scientific Communications, 9:00 to 10:15 AM, SF Marriott Marquis, Golden Gate B

Symposium: The Chemistry of Fermented Beverages (cosponsored by AGFD), 10:00 to 11:30 AM, SF Marriott Marquis, Golden Gate A

Workshop: Chemists Celebrate Earth Day (sponsored by CCA), 10:30 to 11:45 AM

Undergraduate Research Poster Session (cosponsored by CHED, AGFD, ENVR, INOR, MEDI, PHYS, POLY, GEOC, and BIOT), noon to 2:00 PM

Eminent Scientist Lecture with Dr. Carolyn Bertozzi, Stanford University (cosponsored by MEDI), 2:30 to 4:00 PM, SF Marriott Marquis, Golden Gate A

Student Speed Networking with Chemistry Professionals, 4:00 to 5:15 PM

Sci-Mix/Successful Student Chapter Posters, 8:00 to 10:00 PM

Tuesday, April 4

NSF Graduate School Fellowships, 9:00 to 9:45 AM, SF Marriott Marquis, Golden Gate A

Chemistry & the Environment Film Series (cosponsored by CEI), noon to 2:00 PM, SF Marriott Marquis, Golden Gate A

GRADUATE & POSTDOCTORAL SCHOLARS OFFICE. The Graduate & Postdoctoral Scholars Office, with support from the Graduate Education Advisory Board, provides and promotes programs and resources for graduate students and postdoctoral scholars.

Sunday, April 2

ChemIDP™: Planning for Your Career, 11:30 AM to 1:15 PM

Graduate & Postdoctoral Scholars Focus Group, 2:00 to 4:00 PM

Faculty & Postdoc Afternoon Networking Coffee Break, 4:00 to 6:00 PM

Monday, April 3

Student Speed Networking with Chemistry Professionals, 4:00 to 5:15 PM

Graduate & Postdoctoral Scholars Reception, 7:00 to 8:30 PM

For more information about these events and other ACS programs offered to graduate students and postdocs, visit www.acs.org/grad or contact the ACS Graduate & Postdoctoral Scholars Office at graded@acs.org or at 800-227-5558 ext. 4588.

CHEMISTRY TEACHER PROGRAM. The Division of Chemical Education and the ACS Education Division are sponsoring the Chemistry Teacher Program. It will include presentations on current pedagogies, resources, and activities. The 2017 recipient of the James Bryant Conant Award in High School Chemistry Teaching will be a featured presenter during the program. The High School-College Interface Luncheon will bring together educators from all grade levels with the goal of facilitating an exchange of ideas and networking among teachers and professors.

High school and middle school teachers can register for the program directly through Attendee Registration as a pre-college teacher; the reduced registration fee includes program materials, lunch, access to the full ACS meeting, and entry to the exposition. Teachers can receive a certificate documenting up to 24 professional development hours for attending sessions.

Sunday, April 2

Chemistry Teacher Program, 8:30 AM to 4:30 PM

Monday, April 3

High School Polymer Program (cosponsored by POLY), 5:00 to 8:30 PM
For more information, contact the Office of High School Chemistry at education@acs.org or at 800-227-5558 ext. 2105

SOCIAL & TICKETED EVENTS

Friday, March 31

CHAS Laboratory Waste Management
8:00 AM to 5:00 PM, Moscone Center, Room 120

CHAS Laboratory Safety Workshop
8:00 AM to 5:00 PM, Moscone Center, Room 121

Saturday, April 1

CHAS Cannabis Extraction & Analysis Workshop
8:00 AM to 5:00 PM, Moscone Center, Room 120

CHAS How to be a More Effective Chemical Hygiene Officer
8:00 AM to 5:00 PM, Moscone Center, Room 121

CHAS Using ACS Lab Safety Resources in the Classroom
8:00 AM to 5:00 PM, Moscone Center, Room 124

CHAS Reactive Chemical Management for Laboratories & Pilot Plants
8:00 AM to 5:00 PM, Moscone Center, Room 125

COACHing Strong Women in the Art of Strategic Persuasion
8:00 AM to 5:00 PM, SF Marriott Union Square, Sutter 1

COACH: Uping the Game: Refresher Workshop for Past COACh Alums
8:00 AM to 5:00 PM, SF Marriott Union Square, Sutter 2

ACS Presidential Outreach Event — OPEN
Noon to 4:00 PM, Exploratorium, Pier 15

COACh Reception
5:00 to 7:00 PM, SF Marriott Union Square, Russian Hill

Sunday, April 2

Career Pathways Workshops
8:00 AM to 5:30 PM, W San Francisco, Great Room 2

Career Pathways II
8:00 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8:00 AM to 5:30 PM, W San Francisco, Workroom 3

Career Pathways I
8:00 AM to 5:30 PM, W San Francisco, Workroom 1

Undergraduate Hospitality Center
8:00 AM to 5:00 PM, SF Marriott Marquis, Salon 7

Making the Most of Your First National Meeting
8:30 to 9:15 AM, SF Marriott Marquis, Salon 7

Graduate School Reality Check, Part 1: Getting in
10:00 to 11:30 AM, SF Marriott Marquis, Golden Gate Blrm B

Chem Demo Exchange Household Chemicals
11:00 AM to noon, Moscone Center, Hall A

Graduate School Reality Check, Part II: You're in- Now What?
11:30 AM to 12:45 PM, SF Marriott Marquis, Golden Gate Blrm B

ACS Board Luncheon & Meeting
Noon to 1:00 PM, Moscone Center, Gateway Ballroom 103/104

CHED (Division of Chemical Education) High School/College Interface Luncheon/SE-01/$45
Noon to 1:00 PM, SF Marriott Marquis, Salon 7

POLY Board Meeting
Noon to 1:00 PM, Moscone Center, 132

Developing Communication Strategies
Noon to 5:30 PM, Park Central San Francisco, Commonwealth

BIOT Lunch Seminars
12:30 to 2:00 PM, InterContinental San Francisco, InterContinental B

CTA (Committee on Technician Affairs) Awards Luncheon/SE-02/$45
1:00 to 3:00 PM, Hilton SF Union Square, Continental Parlor 3

Networking Social with Graduate School Recruiters
1:00 to 5:00 PM, Moscone Center, Hall A

Networking 101
1:30 to 3:00 PM, SF Marriott Marquis, Golden Gate Blrm A

Graduate & Postdoc Focus Group
2:00 to 4:00 PM, Moscone Center West, 2nd Floor, Area 2

Two-Year to Four-Year College Transfer Survival
2:30 to 3:30 PM, SF Marriott Marquis, Golden Gate Blrm B

Advanced Materials, Technologies, Systems & Processes Plenary Session
3:00 to 6:00 PM, Moscone Center, Gateway Ballroom 103 & 104

McGraw-Hill Education Learning Technologies Workshop
Sponsor: McGraw-Hill Education
3:30 to 6:00 PM, Moscone Center, Room 250

SciBabe: Chemistry Blogging
4:00 to 5:30 PM, SF Marriott Marquis, Golden Gate Blrm A

IAC (Committee on International Activities) Networking Globally: Helping Chemistry Students Find Success in Careers and Study Abroad/SE-03/ no charge
4:00 to 5:30 PM, Hilton SF Union Square, Yosemite C

Faculty and Postdoc Afternoon Coffee Break
4:00 to 6:00 PM, Hotel Nikko San Francisco, Monterey I

Diversity Reception
5:00 to 7:00 PM, Hilton Union Square, Yosemite A & B

AGFD Poster Session Reception
5:00 to 7:00 PM, Moscone Center, West Hall

University of Wisconsin @ Madison Alumni & Friends Social Hour
5:00 to 7:00 PM, Park Central San Francisco, Concordia Park

University of California, San Diego Alumni & Friends
5:00 to 7:00 PM, SF Marriott Marquis, Salon 1

University of Illinois @ Urbana-Champaign Alumni & Friends Reception
5:00 to 8:00 PM, InterContinental San Francisco, Sutter

District I Councilor Caucus
5:30 to 7:00 PM, Hilton SF Union Square, Union Square 1 & 2

CHED Social Reception
5:30 to 7:00 PM, Moscone Center, 134

COLL Social Hour/Poster Session
5:30 to 8:00 PM, Moscone Center, Hall B/C

INOR Poster Session
5:30 to 7:30 PM, Moscone Center, Hall D

ORGN Poster Session
5:30 to 7:30 PM, Moscone Center, West Hall

Joint Research Corporation Petroleum Research Fund Reception in Honor of the Awardee for Research at an Undergraduate Institution
5:30 to 7:30 PM, Hilton Union Square, Golden Gate 4 & 5

International Welcome Reception/ SE-04/no charge
5:30 to 7:30 PM, Hilton Union Square, Grand Ballroom A

District IV Councilor Caucus
6:00 to 7:00 PM, Hilton SF Union Square, Union Square 15 & 16

District V Councilor Caucus
6:00 to 7:00 PM, Hilton SF Union Square, Union Square 17 & 18

District VI Councilor Caucus
6:00 to 7:00 PM, Hilton SF Union Square, Union Square 19 & 20

District II Councilor Caucus
6:00 to 7:00 PM, Hilton SF Union Square, Union Square 3 & 4

District III Councilor Caucus
6:00 to 7:00 PM, Hilton SF Union Square, Union Square 5 & 6

SCHB Entrepreneurs' Poster Session
6:00 to 8:00 PM, Moscone Center, Hall B/C

University of Washington Alumni & Friends/SE-27/$5
6:00 to 8:00 PM, W San Francisco, Great Room 1

Attendee Welcome Reception
6:00 to 8:30 PM, Moscone Center, Halls B/C

CINF Welcoming Reception and Poster Session
6:30 to 8:30 PM, Park Central San Francisco, Franciscan I & II

PROF General Posters
6:30 to 8:30 PM, Moscone Center, Expo Hall B/C

Student Chapter Awards Ceremony
7:00 to 8:30 PM, Hilton SF Union Square, Grand Ballroom B

Analytical Division Poster Session
7:00 to 9:00 PM, Moscone Center, West Hall

MEDI General Posters
7:00 to 9:00 PM, Moscone Center, West Hall

CHED Poster Session
7:00 to 9:00 PM, Moscone Center, Hall D

BIOL Poster Session
7:00 to 9:00 PM, Moscone Center, West Hall

FLUO Poster Session
8:00 to 10:00 PM, Moscone Center, Hall D

Undergraduate Social
8:30 to 11:00 PM, Hilton SF Union Square, Continental Ballroom 1–6

Monday, April 3

Women in the Chemical Enterprise Breakfast/SE-05/$40 (regular)/ SE-06/$20
7:30 to 9:00 AM, Hilton Union Square, Imperial B

YCC Fun run/SE-07/$30 (regular)/ SE-08/$15 (undergraduates)
8:00 to 10:00 AM, Moscone Center West, Outside West Lobby

Career Pathways II
8:00 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8:00 AM to 5:30 PM, W San Francisco, Workroom 3

Career Pathways I
8:00 AM to 5:30 PM, W San Francisco, Workroom 1

Undergraduate Hospitality Center
8:00 AM to 4:00 PM, SF Marriott Marquis, Salon 7

Engaging Colleagues in Dialogue
8:00 AM to noon, Park Central San Francisco, Commonwealth

Improving Scientific Communications
9:00 to 10:15 AM, SF Marriott Marquis, Golden Gate Blrm B

ACS Exposition
9:00 AM to 5:00 PM, Moscone Center, Halls B/C

Teaching Laboratory Safety in the Undergraduate Chemistry Curriculum,
Sponsor: Flinn Scientific Inc.
9:30 AM to noon, Moscone Center, Room 250

Solutions for Innovation
Sponsor: JEOL USA, Inc.
9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 2

Advancing Material Science Research through Spectroscopy
Sponsor: ThermoFisher Scientific
9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 1

Getting Real with Organic Chemistry
Sponsor: CAS
9:30 AM to noon, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 3

CCA Outreach Workshop
10:30 to 11:45 AM, Moscone Center, Hall A

Women Chemists of Color Networking/ SE-09/no charge
10:30 AM to noon, Hilton SF Union Square, Yosemite C

PROF Speaker Luncheon CANCELLED
11:30 AM to 1:30 PM, Hotel Nikko San Francisco, Carmel II

CRC Handbook Discussion Forum
11:30 AM to 3:00 PM, Moscone Center, 134

Committee on Minority Affairs Luncheon/ SE-10/$50 (regular)/ SE-11/$25 (student)
11:30 AM to 1:30 PM, Hilton Union Square, Grand Ballroom A

CHAL (Chemistry & the Law Division) Drug & Power Luncheon/SE-12/$40
Noon to 1:30 PM, Mourad, 140 New Montgomery Street

Undergraduate Research Poster Session
Noon to 2:00 PM, Moscone Center, Hall D

BIOT Lunch Seminars
12:30 to 2:00 PM, InterContinental San Francisco, InterContinental B

How to Make LC Method Development and Peptide Mapping Simpler / Part 2: Tackle Interferences with Advanced Triple Quadrupole Technology
Sponsor: ThermoFisher Scientific
12:30 to 3:00 PM, Moscone Center, Hall B, Exhibitor Workshop Room 1

What can NMR do for the chemist? Introduction to experiments beyond 1D proton and carbon spectra
Sponsor: Bruker
12:30 to 3:00 PM, Moscone Center, Room 250

Leading Change
1:00 to 5:00 PM, Park Central San Francisco, Commonwealth

Graduate and Postdoc Focus Group
2:00 to 5:00 PM, Moscone Convention Center West, 2nd floor, Area 3

Seamless Integration of 2D to 3D SAR to Guide Multi-parameter Optimisation
Sponsor: Optibrium Ltd.
3:30 to 6:00 PM, Moscone Center, Hall B, Exhibitor Workshop Room 1

The Kavli Foundation Emerging Leader in Chemistry Lecture
4:00 to 5:10 PM, Moscone Center, Gateway Ballroom 103/104

Women Chemists Committee Open Meeting and 'Just Cocktails' Reception
4:00 to 5:00 PM, Hotel Nikko San Francisco, Nikko Ballroom II

The Fred Kavli Innovations in Chemistry Lecture
5:15 to 6:30 PM, Moscone Center, Gateway Ballroom 103/104

CHAL Reception
6:00 to 8:00 PM, Jillian's, 175 Fourth Street

CACS (Chinese-American Chemical Society) Dinner Banquet/SE-13/$37
6:30 to 9:00 PM, Far East Café, 631 Grant Avenue

ACS Graduate & Postdoctoral Scholars Reception/SE-14/no charge
7:00 to 8:30 PM, Moscone Center, Room 134

UC Berkeley Dept of Chemistry Alumni & Friends Reception
7:00 to 8:30 PM, InterContinental San Francisco, Grand Ballroom C

Sci-Mix Interdivisional Poster Session (Drink ticket with Registration)
8:00 to 10:00 PM, Moscone Center, Hall D

Tuesday, April 4

University of Minnesota Alumni & Friends Breakfast/SE-16/$5
7:30 to 9:30 AM, Moscone Center, Room 2000

Senior Chemists Breakfast/SE-15/$20
7:30 to 9:30 AM, Hilton SF Union Square, Grand Ballroom A

Career Pathways II
8:00 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8:00 AM to 5:30 PM, W San Francisco, Workroom 3

Career Pathways I
8:00 AM to 5:30 PM, W San Francisco, Workroom 1

Coaching & Feedback
8:00 AM to noon, Park Central San Francisco, Commonwealth

NSF Graduate School Fellowships
9:00 to 9:45 AM, SF Marriott Marquis, Golden Gate Blrm A

ACS Exposition
9:00 AM to 5:00 PM, Moscone Center, Halls B/C

Mass Spec Inlet Versatility to Maximize Productivity
Sponsor: Advion
9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 1

Innovative HPLC Solutions to Increase Efficiency and Productivity in the Lab
Sponsor: Agilent Technologies
9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 2

McGraw-Hill Education Learning Technologies Workshop
Sponsor: McGraw-Hill Education
3:30 PM to 6:00 PM, Moscone Center, Room 250

Women Chemists Committee/Eli Lilly Travel Award Poster Session
11:00 AM to noon, Hilton Union Square, Grand Ballroom A

PROF & SCHB Speaker Luncheon CANCELLED
11:30 AM to 1:30 PM, Hotel Nikko San Francisco, Nikko Carmel II

CINF (Chemical Information Division) Division Luncheon/SE-20/$30
Noon to 1:30 PM, Park Central San Francisco, Franciscan I

COLL (Division of Colloid & Surface) Luncheon/SE-19/$45
Noon to 1:30 PM, W San Francisco, Great Room 1

WCC (Women Chemists Committee) Luncheon/SE-17/$50 (regular)/ SE-18/$25 (student)
Noon to 1:30 PM, Hilton Union Square, Grand Ballroom A

Chemistry & the Environment Film Series
Noon to 2:00 PM, SF Marriott Marquis, Golden Gate Blrm B

BIOT Lunch Seminars
12:30 to 2:00 PM, InterContinental San Francisco, InterContinental B

Advancing HPLC and GC Separations
Sponsor: Agilent Technologies
12:30 to 3:00 PM, Moscone Center, Hall B, Exhibitor Workshop Room 2

Vibrational Spectroscopy for Pharmaceutical Applications
Sponsor: Bruker
12:30 to 3:00 PM, Moscone Center, Hall B, Exhibitor Workshop Room 1

Raman inVia Qontor and LiveTracking
Sponsor: Renishaw
12:30 PM to 3:00 PM, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 3

Leading Without Authority
1:00 to 5:00 PM, Park Central San Francisco, Commonwealth

Local Section Officers, Outreach Coordinator and Speakers Reception
3:30 to 5:30 PM, Hilton SF Union Square, Continental Ballroom 4

Division Officers & Councilors Caucus
4:00 to 5:30 PM, Moscone Center, Room 132

ANYL (Division of Analytical Chemistry) Dinner/SE-21/$25 (regular)/SE-22/$15 (student)
5:00 to 7:30 PM, Hilton SF Union Square, Golden Gate 2

Henry Hill & Lou Sacco Award Reception
5:00 to 7:00 PM, Hotel Nikko San Francisco, Nikko Ballroom III

UCLA Research Showcase
5:00 to 7:00 PM, Moscone Center, Room 135

Sacramento Region Meet & Greet Reception
5:00 to 7:00 PM, W San Francisco, Great Room 1

INOR Poster Session
5:30 to 7:30 PM, Moscone Center, Hall D

ORGN Poster Session
5:30 to 7:30 PM, Moscone Center, Hall D

Moissi Kick-Off Reception
5:30 to 7:30 PM, Hotel Nikko San Francisco, Bay View

Division Officers & Councilors Caucus (DOC/DCC) Reception
5:30 to 6:30 PM, Moscone Center, 133

COMP Poster Session
6:00 to 8:00 PM, Moscone Center, West Hall

ENVR (Division of Environmental Chemistry) Division Reception/SE-23/$20
6:00 to 8:00 PM, Thirsty Bear Brewing Co., 661 Howard St.

NUCL Social Hour
6:00 to 8:00 PM, Moscone Center, 130

CATL Poster Session
6:00 to 8:00 PM, Moscone Center, Hall D

BIOT Poster Session/Social
6:00 to 8:00 PM, Moscone Center, West Hall

ENFL (Division of Energy and Fuel) Awards Dinner/SE-24/$60
6:30 to 9:00 PM, LeColonial, 20 Cosmo Pl.

CELL (Division of Cellulose and Renewable Materials) Awards Banquet/SE-25/$65
6:00 to 10:00 PM, The Chart House, Pier 39, San Francisco, CA 94119

ACS National Awards Banquet Ceremony & General Meeting/SE-26/$130
6:30 to 10:00 PM, SF Marriott Marquis, Salon 8/9

BIOL Poster Session/Social
7:00 to 9:00 PM, Moscone Center, West Hall

Wednesday, April 5

Career Pathways II
8:00 AM to 5:30 PM, W San Francisco, Workroom 2

Career Pathways III
8:00 AM to 5:30 PM, W San Francisco, Workroom 3

Career Pathways I
8:00 AM to 5:30 PM, W San Francisco, Workroom 1

Chemical Forensics International Technical Working Group
8:30 AM to 5:00 PM, Hotel Union Square, Continental Ballroom 4

Electrochemistry 101: Experiments For Use In Undergraduate Labs
Sponsor: Gamry Instruments
9:30 AM to noon, Moscone Center, Room 250

BIOT Lunch Seminars
Noon to 2:00 PM, InterContinental San Francisco, InterContinental B

Structure-Based Drug Design and Ligand Modification
Sponsor: Chemical Computing Group
3:30 to 6:00 PM, Moscone Center, Room 250

POLY/PMSE Lecture & Awards Reception
5:30 PM to 8:00 PM, Moscone Center, 134

ENVR Poster Session
6:00 to 8:00 PM, Moscone Center, Hall D

GEOC Poster Session
6:00 to 8:00 PM, Moscone Center, Hall D

I&EC Poster Session
6:00 to 8:00 PM, Moscone Center, Hall D

PHYS Poster Session
7:00 to 9:00 PM, Moscone Center, Hall D

NUCL Poster Session
7:00 to 9:00 PM, Moscone Center, Hall D

MEDI & ORGN General Poster Social
7:00 to 11:00 PM, Moscone Center, West Hall

WORKSHOPS

The following workshops require a separate registration process and/or entry fee to participate in the event, as indicated in this listing. Participation is open to all interested registrants.

Division of Chemical Health & Safety (CHAS)-sponsored workshop fees (unless otherwise indicated). CHAS member: full registration $375/early registration $300; non-CHAS member: full registration $425/early registration $350. Early registration ends February 17. K–12 science teachers who are American Association of Chemistry Teacher members: $99. Need-based scholarships are available for K–12 science teachers; contact scholarships@labsafetyinstitute.org.

Half-day workshops fees. CHAS member: $175 early registration/$200 after February 17; non-CHAS member: $200 early registration/$225 after February 17.

Registration is required for all CHAS workshops. Register online at dchas.org/workshop-registration-page.

Laboratory Safety—Beyond the Fundamentals. Friday, March 31, 8:00 AM to 5:00 PM. Moscone Center, Room 121. Presenter: James Kaufman. The Laboratory Safety Institute will present a new course at the ACS national meetings which is designed to meet the needs of scientists and science educators wanting to learn more about laboratory safety. "Lab Safety— Beyond the Fundamentals" continues where LSI's introductory course (The Laboratory Safety Workshop) leaves off and explores new areas in lab safety. There is an emphasis on simple and inexpensive steps to create more effective lab safety programs and grow the culture of lab safety.

There is extensive opportunity for questions during the workshop with follow-up by phone and e-mail. This includes a one-hour conference call to help with the implementation of course concepts. Course participants are encouraged to submit in advance five questions or topics they wish to be sure are covered in the course: jim@labsafetyinstitute.org.

Laboratory Waste Management. Friday, March 31, 8:00 AM to 5:00 PM. Moscone Center, Room 120. Presenter: Russ Phifer. CHAS offers this workshop to assist participants with the various regulatory requirements that apply to laboratories that generate hazardous waste, as well as to provide insight into the options for on-site management and off-site disposal. Focus will include discussion on recycling/reclamation techniques, economical handling of waste, and liability issues. There is extensive opportunity for questions during the workshop with follow-up by phone and e-mail.

CANCELLED

Cannabis Extraction Workshop. Saturday, April 1. Moscone Center, Room 120. Presenters: Ezra Pryor, Jahan Marcu, and Melissa Wilcox. 8:00 AM to noon. CHAS and CANN (Cannabis Chemistry Subdivision) present a Cannabis Extraction Workshop, which is a comprehensive review of current methodologies and best practices in the extraction and processing of cannabis. Participants will learn the latest developments in extraction technologies, how to comply with regulations, and how to operate safely. There is extensive opportunity for questions during the workshop with follow-up by phone and e-mail.

CANCELLED

Cannabis Analysis Workshop. Saturday, April 1. Moscone Center, Room 120.Presenters: Ezra Pryor, Jahan Marcu, and Melissa Wilcox. 1:00 to 5:00 PM. CHAS and CANN (Cannabis Chemistry Subdivision) present a Cannabis Analysis Workshop, which is a comprehensive review of current testing requirements, methodologies, and best practices in the analysis of cannabis and cannabis-infused products. Participants will learn how to overcome testing challenges, how to comply with standards, and how to operate safely. There is extensive opportunity for questions during the workshop with follow-up by phone and e-mail.

Reactive Chemical Management for Laboratories & Pilot Plants. Saturday, April 1, 8:00 AM to 5:00 PM. Moscone Center, Room 125. Sponsored by CHAS. Presenters: Neal Langerman and Harry Elston. Chemical reactivity hazards contribute to a significant number of incidents in laboratories and pilot plants. This workshop will provide participants with the knowledge and skill to screen processes for potential hazards, recognize when reactive hazards are present, and implement appropriate controls to reduce the risk of an incident associated with the hazards. Workshop attendees will review case studies of actual incidents and do screening examples in order to understand the screening and recognition process. Group discussions of control methods will allow participants to share their experiences and to evaluate methods for controlling reactivity risks.

How to Be a More Effective Chemical Hygiene Officer. Saturday, April 1, 8:00 AM to 5:00 PM. Moscone Center, Room 121. Sponsored by CHAS. Presenters: Russ Phifer and Jim Kaufman. CHAS offers the How to Be a More Effective Chemical Hygiene Officer workshop to provide participants with a detailed analysis of the CHO position and to prepare for the CHO Certification exam. Participants receive a clear perspective on safety issues in the laboratory, focusing on what the CHO does and how to do it better. The workshop covers the content areas of the certification exam, including a sample test in the same format as the real one. Whether you are a new Chemical Hygiene Officer or an old one, you will find something to put to real use in this fast-paced presentation. There is extensive opportunity for questions during the workshop with follow-up by phone and e-mail.

Using ACS Resources to Teach Lab Safety (replacing Meeting New Chemical Safety Expectation in Instructional Laboratories). Saturday, April 1, 8:00 AM to 5:00 PM. Moscone Center, Room 124. Presenters: Samuella Sigmann and Ralph Stuart. Over the last few years, ACS has released several important new resources and updated others to support teaching laboratory safety at a variety of academic levels from secondary school to undergraduate and research settings. They are built around the RAMP paradigm supported by the ACS Committee on Professional Training guidelines. This two-part workshop will discuss how the ACS publications can be used to support chemical safety education and to promote a proactive safety culture in these settings. Each module, which has separate but complementary content, can be taken individually or both can be taken on the same day.

CANCELLED

Part 1: ACS Safety Tools for Secondary School and Undergraduate Labs. 8:00 AM to noon. This module will use a variety of tools available from ACS to cover topics such as hazard recognition, basic risk assessment, understanding the Globally Harmonized System of Labeling (GHS), selecting personal protective equipment, engineering controls, safe chemical management and storage, and basic chemical waste management principles. The information presented in this module is appropriate for secondary school teachers (including those who are preservice) as well as undergraduate faculty.

CANCELLED

Part 2: ACS Safety Tools for Chemistry Majors and Research Laboratories. 1:00 to 5:00 PM. In 2016, ACS released an updated web version of its *Identifying and Evaluating Hazards in Research Laboratories* document. The methods outlined in this document are designed to address operations in research laboratory settings, which are less defined and more changeable than those in teaching settings. The workshop focuses on the Job Hazard Analysis and Control Banding tools, which are appropriate for most laboratory research at the undergraduate level. Examples of Lessons Learned programs in the research setting will also be reviewed.

CANCELLED

COAChing Strong Women in the Art of Strategic Performance. Saturday, April 1, 8:00 AM to 5:00 PM. San Francisco Marriott Union Square, Sutter 2. Workshop facilitators: Lee Warren and Nancy Houfek. Open to women in academia, industry, national labs, and government. This workshop is designed to provide powerful women with skills to succeed in accomplishing their goals in negotiations and meetings. Participants will be introduced to performance techniques that people in the theater and in leadership training understand about how to be effective, such as body language and nonverbals. They will learn how to articulate a clear purpose, land their message, be heard, enhance personal presence, depersonalize attacks, and manage hot moments. Participants are asked to bring examples of past challenging negotiations or meetings. These moments are examined in the workshop through the use of role plays. Discussion, coaching, and the replay of scenarios creates highly interactive, personal, and powerful learning of the wide range of tactics available for success. Travel assistance is available for women in academia and national labs. Preregister at coach.uoregon.edu. For more information, contact Priscilla Lewis at coach@uoregon.edu.

Upping your Game: Refresher Workshop for Past Workshop Alums. Saturday, April 1, 8:00 AM to 5:00 PM. San Francisco Marriott Union Square, Sutter 1. Workshop facilitators: Barbara Butterfield and Jane Tucker. This workshop is designed to be a refresher of what is learned in COAChing Strong Women in the Power of Strategic Persuasion. It begins with a preview of essential negotiation skills and moves into examination of Cialdini's six principles of influence, dealing with abrasive people, mentoring influence strategies, and dealing with difficult people. Factors contributing to personal success and failure are examined and applied to case studies. You will also be given refresher tools and concepts for making change happen where it needs to happen through exercises and role-plays, learn how to make effective interventions, and get your voice heard at the table. Travel assistance is available for women in academia and national labs. Preregister at coach.uoregon.edu. For more information, contact Priscilla Lewis at coach@uoregon.edu.

ACS CAREER NAVIGATOR

ACS Career Navigator is your home for career services, leadership development, professional education, and market intelligence resources. We offer comprehensive and easily identified tools to help you to achieve your career goals by landing a new job, finding a new career path, comparing your salary, and viewing current trends in the chemistry enterprise to make more informed decisions. Opportunities abound at the ACS national meeting in San Francisco for career development. Take advantage of the resources and tools the ACS Career Navigator offers to help you succeed in the global scientific enterprise.

Are you ready to get started? Refresh your skills and branch into new areas of science and advanced applications with an ACS short course.

Take an ACS Leadership Development System course to gain skills that can be immediately applied in school or on the job.

If you are an ACS member, stop by the ACS Career Fair in the Moscone Center and speak to a career consultant or get a professional head shot taken.

In short, whatever your career goals, the ACS Career Navigator is here to help you achieve and exceed them. We'll see you in San Francisco!

ACS CAREER FAIR

Job seekers, are you looking to jumpstart your job search or enhance your professional development?

Employers, are you looking to hire scientists and engineers? Then you need to attend the ACS Career Fair, open Sunday, April 2, from 6:00 to 8:30 PM; Monday, April 3, from 9:00 AM to 5:00 PM, and Tuesday, April 4, from 9:00 AM to 5:00 PM. The career fair is the place where the best talent and the best employers in chemistry meet.

The ACS Career Fair provides on-site activities for job seekers to help them reach their career goals. ACS will help you prepare for your next career move by providing resources that make it possible to map out your personal job search strategy, strengthen your résumé, and build your interview skills, all with the support of career consultants. During the career fair, participants can take full advantage of the following:

- Networking opportunities
- Résumé reviews
- One-on-one career consulting
- Interview practice and skills building
- More than 30 career-related workshops
- Keynote speakers presented live and via webcast
- Live, on-site interviews on request

The ACS Career Fair is a free event with a national meeting registration. All attendees are free to visit recruiters' booths and drop off their résumés. ACS members interested in a private interview must create a profile and upload their résumés in the ACS Career Fair database. The ACS Career Fair will be held in conjunction with the ACS National Exposition, Sunday through Tuesday.

Please note: We cannot guarantee that you will secure interviews at the ACS Career Fair. Interviewing is strictly contingent on the availability of positions and the credentials and qualifications that employers are seeking.

One-on-one career consulting. Individual 30-minute appointments with career consultants are available both on-site and online. These consults can help you strengthen your résumé, improve your interviewing skills, and design a job search or comprehensive professional growth strategy. Please bring a copy of your résumé or CV to all appointments. All one-on-one on-site career consulting sessions will take place in the Résumé Review/ Mock Interview area in the Moscone Center. Sign-up begins at 9:00 AM on Sunday, April 2, on a first-come, first-served basis.

Career and professional development workshops. More than 20 career-related workshops will help you with everything from improving your résumé to optimizing job performance or acing an interview. Workshop times are subject to change. Please consult the online workshop schedule at www.acs.org/careerfair for locations.

Sunday, April 2

New Technologies to Find Jobs and Manage Your Career, 10:00 to 11:30 AM

ChemIDP: Planning for Your Career, 11:30 AM to 1:15 PM

Setting Yourself Up for Success in an Interview, 1:00 to 3:00 PM

Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 1:00 to 3:00 PM

Finding Yourself: Identifying a Career That Matches Your Strengths and Values, 1:00 to 4:00 PM

Foreign National Scientist Obtaining a Job in the US, 1:30 to 3:00 PM

Writing Excellent Proposals, 3:30 to 5:00 PM

Making the Most of Your Interview: Outshine the Competition, 3:30 to 5:30 PM

Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 3:30 to 5:30 PM

Networking: How to Get Started, 4:30 to 5:30 PM

Monday, April 3

Opportunities for Chemists in the Federal Government, 8:00 to 10:00 AM

Working in Higher Education, 8:00 AM to noon

Working for Yourself, 8:00 AM to noon

How to Find and Apply for a Chemistry Position in the Federal Government, 10:30 AM to 12:30 PM

Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 1:00 to 3:00v PM

Setting Yourself Up for Success in an Interview, 1:00 to 3:00 PM

Finding Yourself: Identifying a Career that Matches your Strengths and Values, 1:00 to 4:00 PM

Making the Most of Your Interview: Outshine the Competition, 3:30 to 5:30 PM

Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 3:30 to 5:30 PM

Networking: How to Get Started, 4:30 to 5:30 PM

Tuesday, April 4

Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 8:00 to 10:00 AM

Setting Yourself Up for Success in an Interview, 8:00 to 10:00 AM

Finding Yourself: Identifying a Career That Matches Your Strengths and Values, 8:00 to 11:00 AM

Making the Most of Your Interview: Outshine the Competition, 10:30 AM to 12:30 PM

Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 10:30 AM to 12:30 PM

Networking: How to Get Started, 11:30 AM to 12:30 PM

Opportunities for Chemists in the Federal Government, 1:00 to 3:00 PM

Working for Yourself, 1:00 to 5:00 PM

Working in Higher Education, 1:00 to 5:00 PM

How to Find and Apply for a Chemistry Position in the Federal Government, 3:30 to 5:30 PM

Wednesday, April 5

Careers in Industrial Chemistry: Identifying Your Role in the Industrial Value Chain, 8:00 to 10:00 AM

Setting Yourself Up for Success in an Interview, 8:00 to 10:00 AM

Finding Yourself: Identifying a Career That Matches Your Strengths and Values, 8:00 to 11:00 AM

Making the Most of Your Interview: Outshine the Competition, 10:30 AM to 12:30 PM

Résumé Development: Marketing Your Brand for an Industrial Chemistry Position, 10:30 AM to 12:30 PM

Networking: How to Get Started, 11:30 AM to 12:30 PM

Employers—Find the talent you need at the ACS Career Fair. Leading employers around the world trust and depend on ACS to provide them with the talent they need to innovate and excel. At our most recent event, approximately 1,000 global job seekers—from recent grads to seasoned professionals—met with recruiters seeking to fill positions in all facets of chemistry, pharmaceuticals, and biotechnology.

The ACS Careers Database can help manage your employer account, post jobs, search for qualified candidates, and schedule career fair interviews. Moreover, participating in the ACS Career Fair enables you to accomplish the following:

- Connect with top talent via on-site interviews.
- Screen candidates, and make appointments in advance.
- Find the personnel your company needs to thrive, from entry- to executive-level positions.
- Meet qualified candidates informally via networking forums.
- Extend your presence for 30 days after the career fair via the ACS jobs database.

Looking for a more traditional career fair experience? Employers can purchase booth space inside the exposition hall, enabling your company to maximize its ability to showcase products and services and connect with job seekers. Employers can sign up for the ACS Career Fair Recruiters Row package online at www.acs.org/careers.

Employers will receive an e-mail confirmation and must visit the ACS Career Fair Information Booth to pick up their blue badge. For more information, please visit www.acs.org/careerfair. You can also contact Heather McNeill at 202-452-8918 or e-mail her at h_mcneill@acs.org.

ACS SHORT COURSES

The following short courses, specifically designed to improve the skills and marketability of chemical scientists and technicians, are offered in conjunction with the national meeting. ACS member, early registration, and group discount rates are available. A course fee and registration sepa-

rate from the national meeting are required. For more information on ACS Short Courses, to obtain pricing details, or to view a full course catalog, visit www.proed.acs.org. If youhave questions, call 202-872-4508, fax 202-872-6336, or e-mail proed@acs.org

ANALYTICAL

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, April 1–2

Fundamentals of High-Performance Liquid Chromatography, April 3–4

BIOLOGICAL/PHARMACEUTICAL/ MEDICINAL CHEMISTRY

Application of Pharmacokinetics & Safety Pharmacology for Chemists in Drug Development, April 2

COMPUTERS/STATISTICS/ ENGINEERING

Chemical Engineering for Chemists, April 1–2

Statistical Analysis of Laboratory Data, April 2–4

ORGANIC/PHYSICAL CHEMISTRY

1-D & 2-D NMR Spectroscopy: Structure Determination of Small-Molecule Organic Compounds, April 1–2

Dispersions in Liquids: Suspensions, Emulsions & Foams, April 2–3

Organic Synthesis: Methods & Strategies for the 21st-Century Chemist, April 4–5

POLYMER CHEMISTRY

Polymeric Coatings, April 1–2

Polymer Science & Technology, April 1–2

PROFESSIONAL DEVELOPMENT

Effective Technical Writing, April 4–5

Chemistry for Non-Chemists: The Basics, Language, and Function of Chemistry, April 2

Write Your Own Patent Applications, April 2

REGULATORY/ENVIRONMENTAL

Intellectual Property Strategies for Technical Professionals, April 2

Methods Development, Validation Procedures & Regulatory Compliance Issues, April 3–4

Write Your Own Patent Applications, April 2

Highlights of FDA and Other cGMP Regulations, April 5

2017 LEADERSHIP DEVELOPMENT SYSTEM COURSE OFFERINGS

Whether you are a manager, experienced professional, or new to the workforce, we invite you to attend an ACS Leadership Development System course held at the ACS national meeting. The following four-hour facilitated courses require a fee of $150 each for ACS members and $300 each for nonmembers. Register for these courses when you register for the meeting. For more information and full course descriptions, visit www.acs.org/leadershipdevelopment.

Engaging Colleagues in Dialogue. Monday, April 3, 8:00 AM to noon. Engaging Colleagues in Dialogue is a four-hour, hands-on interactive course that helps you develop your one-on-one communication skills. You will learn how to improve both sides of the communication exchange: first working to understand how to better communicate your messages, and second working on listening and acknowledging others' messages. You will even have an opportunity to assess your own communication skills through conversations with colleagues.

Developing Communication Strategies. Sunday, April 2, 1:00 to 5:00 PM. With the skills that you'll gain from this half-day workshop, you'll be a better communicator in your role as an ACS leader and as a leader in your workplace and in your community. Working in small interactive groups, you'll have the chance to develop and practice your own effective communication strategy. Plan to attend this workshop and discover how a comprehensive communication strategy can make both your goals and the goals of ACS possible.

Leading Change. Monday, April 3, 1:00 to 5:00 PM. If you are involved in shifting team priorities, changing the direction of a project, or reconfiguring teams, understanding how people react to change and how to help yourself and others effectively deal with the changes is key to increasing your professional success.

Coaching and Feedback. Tuesday, April 4, 8:00 AM to noon. This hands-on, four-hour course will provide you with a proven process and practical tools to help coach team members, project groups, employees, and volunteers more regularly and effectively. As a participant, you will work on real coaching opportunities to help you practice addressing the development and performance issues you have identified.

Leading Without Authority. Tuesday, April 4, 1:00 to 5:00 PM. Whether in a lab, the office, the classroom, or on a volunteer committee, you will likely find yourself leading others without formal or "positional" authority and need to be able to influence them to accomplish the project. This four-hour interactive workshop provides practical tools to help you gain cooperation and engage others in accomplishing project and team goals.

EXHIBITOR SPONSORED WORKSHOPS

Exhibiting companies will host free education sessions for attendees to introduce new products and services, build skills with specific tools and techniques, and highlight applications for existing instrumentation. Visit www.acs.org/sanfran2017 to register for workshops.

Sunday, April 2

McGraw-Hill Education Learning Technologies Workshop. *Sponsor:* McGraw-Hill Education, 3:30 to 6:00 PM, Moscone Center, Room 250.

3:30 to 4:30 PM. Tactics for Facilitating Flipped Learning— Dr. Danae Quirk Dorr, Minnesota State University, MankatoDuring this workshop, participants will actively explore various strategies that may be utilized in building a student need-based flipped learning environment. By the end of the workshop, participants should be equipped

with tools that they can incorporate into their own classrooms to help bridge content delivery and assessment of student learning.

4:45 to 6:00 PM. Using ALEKS as a Tool for General Chemistry Preparation and Blended Instructional Design—Dr. Tracy McGill, Emory University

Monday, April 3

Solutions for Innovation. *Sponsor:* JEOL, USA, Inc., 9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 2.

Ambient Ionization Mass Spectrometry, Scanning Electron Microscopy.

NMR Structure. Learn how the latest innovations from JEOL integrate together to enhance your science.

Getting Real with Organic Chemistry. *Sponsor:* CAS, 9:30 AM to noon, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 3.

Students are often left wondering—why should I care? How does this apply to me and my future career? Professors are tasked with trying to connect the real world with the concepts taught in textbooks. Come hear how Chemistry Class Advantage™, a new digital learning solution from CAS, will help you teach the relevance of organic chemistry, as well as bridge the gap between memorization and conceptual understanding.

Advancing Material Science Research through Spectroscopy. *Sponsor:* Thermo Fisher Scientific, 9:30 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 1. New materials present new analytical challenges. Like many labs today, you need to stay ahead of the curve. This workshop will show you how FTIR and Raman spectroscopy can be applied in your lab; from the discovery of new materials, to solving production problems and assuring product quality. Industry expert will guide you through the latest trends and techniques to solve your toughest challenges.

How to Make LC Method Development and Peptide Mapping Simpler/Part 2: Tackle Interferences with Advanced Triple Quadrupole Technology. *Sponsor:* Thermo Fisher Scientific, 12:30 to 3:00 PM, Moscone Center, Hall B, Exhibitor Workshop Room 1. Part I: How to Make LC Method Development and Peptide Mapping Simpler Abstract: Why should method development and peptide mapping be a challenge? Come and see how the latest developments in UHPLC afford method transfer from any LC with higher levels of reproducibility as well as resolution, and how when it comes to peptide mapping, we haven't just revolutionized one part of your workflow, we have revolutionized them all!

Part II: Title: Tackle Interferences with Advanced Triple Quadrupole Technology

Abstract: Kick interference to the curb, achieve better detection limits and maximize lab efficiency in the face of any sample matrix. Challenging applications are no match for new triple-quadrupole ICP-MS technology with unprecedented interference removal capabilities.

New Reaxys: Help Shape the Future of Chemistry Search. *Sponsor:* Elsevier, 12:30 to 3:00 PM. Moscone Center, Hall C, Exhibitor Workshop Room 4. The Reaxys/Elsevier team invites you to join this session to help share your experiences and thoughts on what makes the ideal chemistry search. Combining a mix of pre-defined testing, surveys and an open discussion, the product team would like to get your perspective on what makes a good search and discovery experience throughout your chemistry research workflow. Apply your real-life experiences to this session and help shape the future of chemistry search. We look forward to seeing you there.

Wiley Workshop: Technology in the Modern General Chemistry Classroom. *Sponsor:* Wiley, 12:30 to 3:00 PM, Moscone Center, Hall B, Exhibitor Workshop Room 2. Please join Wiley as we explore the trends and challenges of teaching general chemistry utilizing technology. Collaborate with your peers on what's working well and what's needed to improve student engagement and performance in this course.

Share your feedback on a forthcoming, digital general chemistry project from Jason Kautz, University of Nebraska- Lincoln. Lunch will be served! We look forward to seeing you in San Francisco.

Seamless Integration of 2D to 3D SAR to Guide Multi-parameter Optimisation. *Sponsor:* Optibrium, 3:30 to 6:00 PM, Moscne Center, Hall B, Exhibitor Workshop Room 1. This hands-on workshop in collaboration with BioSolveIT will explore how the combination of 2D structure activity relationships (SAR) with 3D structure-based design can be used to guide the optimisation of novel, high-quality compounds. Practical examples will be illustrated using both Optibrium's StarDrop and BioSolveIT's SeeSAR software

Teaching Laboratory Safety in the Undergraduate Chemistry Curriculum. *Sponsor:* Flinn Scientific, Inc., 9:30 AM to noon, Moscone Center, Room 250. Many faculty and lab managers at undergraduate institutions often find it difficult to incorporate laboratory safety throughout their courses. Join us as we discuss how to integrate Flinn Scientific's new engaging online student laboratory safety course and other valuable safety resources into your curriculum and learn how these resources can be used to build a positive safety culture in your department and school.

What can NMR Do For The Chemist? Introduction to Experiments Beyond 1D Proton and Carbon Spectra. *Sponsor:* Bruker, 12:30 to 3:00 PM, Moscone Center, Room 250. With the modern NMR hardware and software available today, many of the experiments that used to be considered complicated and unnecessary are now quite routine and extremely beneficial to the chemist. This workshop will present an introduction to the alphabet soup of NMR experiments and explain what they are, what information can be obtained from them, and when to use one over another.
Topics will include:

- 2D experiments commonly used for structure verification and elucidation such as COSY, TOCSY, HSQC, and HMBC.
- Examination of NMR active nuclei that might be of interest to the inorganic chemist and important things to consider when running these experiments.
- Brief introduction to Magic Angle Spinning (HR-MAS and MAS) methods
- Quick look into the possibilities of triple resonance bio-molecular NMR.

McGraw-Hill Education Learning Technologies Workshop. *Sponsor:* McGraw-Hill Education, 3:30 to 6:00 PM, Moscone Center, Room 250.

3:30 to 4:30 PM. Implementing Connect and its Adaptive Learning Tools in the General Chemistry Classroom—Dr. Jason Overby, College of Charleston. While the online homework paradigm has been a regular component of

chemistry instruction for many years, the addition of adaptive learning tools presents a new challenge to instructors. This workshop will provide an overview of the ways that Connect and its adaptive learning tools can effectively incorporated into any general chemistry classroom.

4:45 to 6:00 PM. The Many Faces of ALEKS in General and Elementary Chemistry at the University of Toledo—Dr. Andy Jorgensen, University of Toledo

University of Toledo has utilized assessment and learning technology to better place students into introductory chemistry courses, as well as increase mastery and retention throughout those introductory courses. During this session, Professor Jorgensen will share their implementation details, results, and overall experience

Tuesday, April 4

Mass Spec Inlet Versatility to Maximize Productivity. *Sponsor:* Advion, 9:30 AM to noon, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 1. With the daily need to analyze liquids, solids, vapor-phase compounds and even air-sensitive samples, the ability to change sample inlets is indispensable. Learn how a single instrument can be adapted to each of these sample requirements and rapidly changed to accommodate back-to-back assays. Listen to users in the field speak about the innovative sample inlets that have cut down on prep and streamlined their everyday work flow.

Innovative HPLC Solutions to Increase Efficiency and Productivity in the Lab. *Sponsor:* Agilent Technologies, 9:30 AM to noon, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 2. This workshop will focus on 2 topics: Increasing productivity of biotherapeutic characterization in drug development and developing rapid HPLC methods with sufficient resolution and speed. Detailed discussion utilizing novel HPLC instrumentation, software, and column chemistries will be discussed— with time for Q&A with Agilent Application Scientists.

Engaging Millennials in the Classroom: A Panel Discussion with Dr. Neil Garg. *Sponsor:* Top Hat, 11:00 AM to noon, Moscone Center, Hall B, Exhibitor Workshop Room 3. With millennials demanding a more engaging learning experience, higher education instructors have had to evolve their teaching methods. Through this lively panel discussion moderated by Dr. Neil Garg, hear about tips and tricks that experts in the field are using to foster active learning both inside and outside the classroom.

Raman inVia Qontor and LiveTracking. *Sponsor:* Renishaw, 12:30 to 3:00 PM, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 3. inVia Qontor—Accurate Raman imaging of rough samples and/or those with complex surface topographies, now even faster with the new Renishaw ultra-fast Centrus detector.

Advancing HPLC and GC Separations. *Sponsor:* Agilent Technologies, 12:30 to 3:00 PM, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 2. QbD solutions for analytical method development in HPLC: Real-world data will be presented demonstrating unique ways to overcome analytical challenges. Plus, Agilent will provide an introduction to modern 2D-HPLC across multiple sample types. See the latest developments on this exciting work-flow that you can implement today. Plus witness a new era in Gas Chromatography, the Intuvo 9000 GC. Resolve Your Search for More Ions by discovering the advantages of Agilent's GCMS solutions.

Vibrational Spectroscopy for Pharmaceutical Applications. *Sponsor:* Bruker, Tuesday, 12:30 to 3:00 PM, Moscone Center, Exhibit Hall B, Exhibitor Workshop Room 1. The latest advances in the FT-IR and Raman instrumentation and applications will be reviewed on this seminar with a thorough discussion of the following topics:

- Contaminations in pharmaceutical products
- Reverse engineering
- Structural changes in proteins
- Maximization of protein stability
- Chemical imaging of biological tissues

Examples of applications will include analysis of proteins secondary structure, protein melting point determination, bacteria recognition, analysis of tablets. Seminar will include live demonstration of new Bruker FTIR microscope and hands-on session. Attendees are encouraged to bring samples of interest for analysis during the hands-on session.

Wednesday, April 5

Electrochemistry 101: Experiments For Use In Undergraduate Labs. *Sponsor:* Gamry Instruments, 9:30 AM to noon, Moscone Center, Room 250. Gamry Instruments has developed a complete laboratory course in electrochemistry for undergraduate facilities. The course includes experiments designed to engage the students and provide them the opportunity to explore various disciplines in chemistry; such as, analyte characterization, aqueous sample testing, digital simulations, electrosynthesis, sensors, batteries, and corrosion. The complete educational bundle includes the instrument, teaching and student manuals with eleven separate experiments, as well as all cells and electrodes needed to complete a semester course for 20 students. This workshop will be an introduction to all aspects of the course material via the performance of select experiments.

Structure-Based Drug Design and Ligand Modification. *Sponsor:* Chemical Computing Group, 3:30 to 6:00 PM, Moscone Center, Room 250. The course covers MOE applications for interactive structure based design. Examples include active site visualization, protein-ligand contact analysis and ligand modification/optimization in the receptor pocket. Conformational searching and analysis of the ligand to assess ligand flexibility will be discussed. A protocol for aligning and superposing protein complexes in the context of protein selectivity will be studied.

SPEAKER INSTRUCTIONS

ALL SPEAKERS and poster presenters must register and pay the appropriate registration fee to attend the meeting. Invited speakers should contact their symposium organizer or division program chair to clarify terms of their invitation.

As a speaker, you should prepare for your presentation by verifying the following details: the status of your abstract at abstracts.acs.org (using your ACS ID to log in to the system); mode of presentation (oral or poster); and the time, length, and location of your presentation. You should arrive in your presentation room at least 30 minutes before your scheduled speaking time. Poster presenters should set up posters at least one hour before the start of the poster session. If you need to withdraw your presentation, please send a withdrawal notice to maps@acs.org and contact your symposium organizer immediately.

TECHNICAL SESSION EQUIPMENT. Each technical session meeting room will be equipped with the following: LCD projector, screen, podium, podium microphone or lapel microphone, and laser pointer. As a speaker, you will need to provide your own laptop or arrange for specialty equipment directly with your symposium organizer and/or division program chair. To request other specialty equipment (at the standard fee), contact an ACS Operations Office during the meeting.

SPEAKER READY ROOMS & AUDIOVISUAL SERVICE CENTERS. As a presenter, you may use the speaker ready rooms to preview your presentation, ensure compatibility with our LCD projectors, or fulfill last-minute audiovisual equipment orders. We strongly recommend that all presenters come to the speaker ready room the day before their presentation to check for connectivity and resolution. The hours of operation will be from 3:00 to 5:00 PM Saturday and 7 AM to 6 PM Sunday through Thursday. Visit the ACS Operations Office at any ACS property for speaker ready room locations. Speaker ready rooms are not equipped with copy machines. There are business centers located in each building of the Moscone Center that provide a range of services including copying, incoming and outgoing faxes, computer access, laser printing, and shipping: in the North Hall on the lower level under the escalators, adjacent to Room 130; in the South Hall, on the lower level, adjacent to Hall C; and in the West Hall, on the lobby level near the Howard St. entrance.

POSTER SESSIONS. All materials must be confined to a 4-foot-high by 8-foot-wide display board in the convention center and a 4-foot-high by 6-foot-wide display board in hotels. Presenters must mount their poster one hour before the scheduled session start time. Poster numbers supplied by ACS will be in the upper corner of each poster board; this number corresponds with the number assigned to each poster in the technical program. Pushpins will be available at the poster session. Presenters must remain with their posters for the duration of their scheduled session as indicated in the technical program. All posters must remain up until the session ends and then must be removed within one hour. ACS cannot assume responsibility for materials beyond these time limits.

SCI-MIX POSTER SESSION ONLY. Sci-Mix presenters may begin poster setup at 7:15 PM (45 minutes before the session begins). Each presenter may be accompanied by one assistant only, and both people are required to arrive together when entering the hall. After exiting, presenters will not be permitted to reenter the hall until the session begins at 8:00 PM.

ABSTRACTS & PREPRINTS

ONLINE TECHNICAL PROGRAM. The technical program for the 253rd ACS National Meeting is now available at www.acs.org/sanfran2017. You can search by divisions or committees, symposia, speakers, or keywords from abstracts as well as presidential events and the multidisciplinary theme of "Advanced Materials, Technologies, Systems & Processes."

ABSTRACTS (USB FLASH DRIVE). Abstracts of all scientific sessions at the meeting can be purchased in USB flash drive (thumb drive) format through ACS Attendee Registration either online before February 20 or on-site in San Francisco from April 2–6. The ACS member fee is $65 each; the nonmember fee is $90 each. Attendees can pick up their abstracts on-site at ACS Attendee Registration at the Moscone Center. You can have a USB flash drive shipped to you if you place your order before February 20, pay an $8.00 postage fee per item, and provide a valid street address within the U.S. If you are not attending the meeting, you can purchase abstracts only from the ACS Office of Society Services, 1155 16th St. N.W., Washington, D.C. 20036; 800-227-5558. Abstract USB flash drives and their shipping costs are nonrefundable.

GRAPHICAL ABSTRACTS. Graphical abstracts from the polymer chemistry division may be ordered directly from the division. You can purchase them by e-mailing Kathy Mitchem (kathyl@vt.edu) or inquiring about these products at the hospitality table for the division near their meeting rooms.

TECHNICAL PROGRAM SUMMARY

Presidential Events — PRES

A. Campbell, Program Chair

San Francisco Marriott Marquis/ Moscone Center	S	M	Tu	W	Th
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal **	PE				
Science for a Sustainable Energy Future **		D			
PHYS Division Awards Symposium *(PHYS)	D	D	D	A	
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Best Practices in Selecting & Presenting Safety Training Content *(CHAS)	P				
ACS Award in the Chemistry of Materials: Symposium in Honor of Douglas A. Keszler *(INOR)	E		D		
Celebrating 90 years of the WCC: Reflections of Past Chairs *(WCC)		A			
Chemical Forensics *(ANYL)		D	D		
Excellence in Graduate Polymer Research *(POLY)		D	DE		
Teaching, Researching & Community Building in the Global Chemical Enterprise *(IAC)		D			
Rising Star Award Symposium *(WCC)		P			
Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators *(PROF)			A		
GSSPC: Water Sustainability *(CHED)			D		
Communicating Science in the 21st Century to Diversified Audiences *(CHED)				D	
What Have We Learned & Where Are We Going: Post-Settlement in the University of California *(CHAS)				D	
Current Best Practices for Chemistry REU Programs *(CHED)					A

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.
**Primary organizer of a cosponsored symposium.

AMTSP: Advanced Materials, Technologies, Systems & Processes
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E = EVE DE = AM/PM/EVE PE = PM/EVE

Multidisciplinary Program Planning Group (continued) — MPPG

K. Beers, Program Chair

Moscone Center	S	M	Tu	W	Th
Spotlight on Advanced Materials, Technologies, Systems & Processes in the *Journal of the American Chemical Society*	A				
Advanced Materials, Technologies, Systems & Processes Plenary Session	P				
Advanced Materials, Technologies, Systems & Processes: Implementation of Chemistry into Practice		A			
The Kavli Foundation Emerging Leader in Chemistry Lecture		P			
The Fred Kavli Innovations in Chemistry Lecture		P			
Nanoscience & Nanotechnology for Advanced Materials & Technologies		P			
Next Generation Smart Materials *(POLY)	A	D	D	D	A
Catalysis for Unconventional Energy Sources *(ENFL)	D	A			
Polymeric Materials for Performance & Sustainability *(POLY)	D	D	AE	D	A
Catalytic Materials from Molecular Insight *(COMP)	D	D	D		
Advanced Materials & Technologies for Solar Energy Conversion & Storage *(ENFL)	D	D	D		
Computations for CO_2 Capture, Conversion & Sequestration *(ENFL)	D	D			
Janus Particles: Synthesis, Characterization & Applications *(PMSE)	D	D			
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Incorporating Polymer Science into the Classroom *(POLY)	D				
Innovative Chemistry & Materials for Electrochemical Energy Storage *(ENFL)	P	D	D	D	A
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
ACS Award in the Chemistry of Materials: Symposium in Honor of Douglas A. Keszler *(INOR)	E		D		
Support & Activator Effects on Metal-Mediated Polymerization *(PMSE)		D	D		
50th Anniversary Celebration of Macromolecules *(POLY)		D			
Science for a Sustainable Energy Future *(PRES)		D			
Industrial Innovations in Polymer Chemistry *(POLY)		P			

Multidisciplinary Program Planning Group — MPPG

K. Beers, Program Chair

Moscone Center	S	M	Tu	W	Th
Chemistry Is Central to Applied Materials *(INOR)			AE	A	
Functional Porous Materials for Sustainable Energy *(ENFL)			D	D	A
Biomass & Biofuel Processing *(ENFL)			D	D	
Polymers Under Deformation *(PMSE)			D	D	
State-of-the-Art Methods for Modeling Materials Chemistry *(COMP)			D	D	
Polymer Chemistry (RSC) Lectureship *(POLY)			D		
Advances in Polysaccharides: Practice & Applications *(CELL)			P	D	D
Undergraduate Laboratory Experiments Involving Advanced Materials *(CHED)				D	
Frontiers in Glycoanalytics *(CELL)				P	A
Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry *(CELL)				P	D

Division of Agricultural & Food Chemistry — AGFD

N. Seeram, Program Chair

Hilton San Francisco Union Square	S	M	Tu	W	Th
Chemistry & Biological Effects of Maple Food Products	D				
Chemistry of Korean Foods & Beverages **	D				
Withycombe–Charalambous Graduate Student Symposium **	P				
General Posters	E				
Structure & Chemistry of Proteins of Food Safety & Food Manufacturing Interest		A			
Artisanal Foods AMTSP		D	A		
Chemistry & Biological Activities of Phenolic Compounds from Fruits & Vegetables		D	D	D	
General Papers		P	P	D	D
Sci-Mix		E			
Chemistry of Tree Nuts			D		
Bliss Point: Food Satiety & Food Mood Effects				A	
Chemistry of Cellulosic Natural Products				P	
Synthetic Biology in Food & Agriculture					A
Coffee & Cocoa Products					D
Nanocellulose Processing & Analysis *(CELL)	D	D			

Division of Agricultural & Food Chemistry — AGFD

N. Seeram, Program Chair

Hilton San Francisco Union Square	S	M	Tu	W	Th
Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems *(CELL)	D	P	D	D	D
Undergraduate Research Posters *(CHED)		P			
Developments in the Fields of Celluloses & Lignocelluloses: In Honor of Dr. Rajai Atalla *(CELL)			D	D	D
Advances in Polysaccharides: Practice & Applications *(CELL)			P	D	D
Biobased Gels & Porous Materials *(CELL)				D	D
Advances in Resource Recovery & Conservation in Water Systems *(ENVR)				PE	D

Division of Agrochemicals — AGRO

S. Jackson, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Contaminants of Emerging Concern in Natural & Engineered Systems *(ENVR)	D	D		E	
Hollyweird Chemistry *(CPRC)	P	D			
Contaminants in Urban & Coastal Estuarine Ecosystems *(ENVR)				PE	D

Division of Analytical Chemistry — ANYL

L. Baker, K. Phinney, Program Chairs

Hilton San Francisco Union Square	S	M	Tu	W	Th
Synthesis & Characterization of Materials for Energy Applications ** AMTSP	D	D	D	D	
Coherent Multidimensional Spectroscopy in Materials Science ** AMTSP	D	D			
Advances in Separations	D				
Analytical Neuroscience	D				
New Analytical Advances in Accelerator Mass Spectrometry (AMS)	D				
Analytical Division Poster Session	E				
ACS Award in Chromatography: Symposium in Honor of Robert T. Kennedy		A			
Chemical Forensics **		D	D		
Biomedical Advances in Cancer Detection & Therapeutics Using Advanced Analytical Techniques		D			
ACS Award in Analytical Chemistry: Symposium in Honor of Donald F. Hunt		P			

Division of Analytical Chemistry — ANYL

L. Baker, K. Phinney, Program Chairs

Hilton San Francisco Union Square	S	M	Tu	W	Th
Sci-Mix		E			
Metamorphosis of Supercritical Fluid Chromatography to Chromatographic Systems Using Carbon Dioxide			A		
Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of David R. Walt **			A		
Advanced Materials, Discovery, Characterization & Safety			D		
New Applications of Supercritical Fluid Chromatography			P		
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement: Symposium in Honor of Vicki H. Wysocki **			P		
Hierarchical Characterization of Materials Using Atomic Spectrometry & Related Techniques AMTSP				A	
Active Learning in the Undergraduate Analytical Chemistry Curriculum **				D	
Recent Innovations in Nano-Biosensing				D	
Applications of Wearable or Implantable Sensors for Systems in Biology AMTSP				P	D
Advances in Analytical Electrochemistry					D
Advances in Analytical Mass Spectrometry					D
Advances in Analytical Spectroscopy					D
Accurate Mass/High-Resolution Mass Spectrometry for Environmental Monitoring & Remediation *(ENVR)	D	A		E	
Contaminants of Emerging Concern in Natural & Engineered Systems *(ENVR)	D	D		E	
Nanocellulose Processing & Analysis *(CELL)	D	D			
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Separation of Macromolecules & Particulates *(POLY)	D				
Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences *(ENVR)		P		E	
Undergraduate Research Posters *(CHED)		P			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer *(I&EC)		P			
Developments in the Fields of Celluloses & Lignocelluloses: In Honor of Dr. Rajai Atalla *(CELL)			D	D	D
Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies *(ENFL)			D	D	
Frontiers in Glycoanalytics *(CELL)				P	A

Division of Biochemical Technology — BIOT

M. O'Malley, V. Roy, Program Chairs

InterContinental San Francisco	S	M	Tu	W	Th
Biosimilars	A				
David Perlman Memorial Lectureship	A				
Biophysical & Biomolecular Processes AMTSP	D	D	D	A	
Upstream Processes AMTSP	D	D	D	D	A
Downstream Processes AMTSP	D	D	D	D	D
Biobased Products	D	D	D	P	
Start-up Road AMTSP	E	D			
Emerging Technologies AMTSP		A	D	D	A
James M. Van Lanen Distinguished Service Award & Marvin J. Johnson Award in Microbial & Biochemical Technology		A			
Sci-Mix		E			
W. H. Peterson Awards & BIOT Young Investigator Award			A		
Poster Session AMTSP			E		
Alan S. Michaels Award in the Recovery of Biological Products			E		
Quality by Design				A	D
2017 E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Eleftherios T. Papoutsakis **				A	
Drug Product & Delivery				D	D
D.I.C. Wang Award Lecture				E	
Biotechnology & Bioengineering Elmer Gaden Award Lecture					A
Biotechnology & Bioengineering Daniel IC Wang Award					E
Cellulose Structure & Biosynthesis *(CELL)	D	D	A		
Science for a Sustainable Energy Future: Energy Storage *(PRES)		D			
Undergraduate Research Posters *(CHED)		P			
Kathryn C. Hach Award for Entrepreneurial Success: Symposium in Honor of David R. Walt *(ANYL)			A		

Division of Biological Chemistry — BIOL

L. Hedstrom, Program Chair

Moscone Center	S	M	Tu	W	Th
Graduate Student & Postdoctoral Fellow Symposium	A			P	A
Ronald Breslow Award for Achievement in Biomimetic Chemistry: Symposium in Honor of Benjamin G. Davis	A				
ACS Award in Pure Chemistry: Symposium in Honor of Neal K. Devaraj	P				
Goodman Award: Symposium in Honor of Jennifer Doudna	P				
Current Topics in Biochemistry	E		E		
Early Career Investigators in Biological Chemistry		A			
Nucleic Acid Therapeutics: Mechanisms & Applications		D			
Sci-Mix		E			
Metalloprotein-Initiated Signaling Transduction Response to Redox Stress **			A		
Chemical Epigenetics			A		
ACS Chemical Biology Award Symposium **			P		
Mid-Career Investigators in Biological Chemistry				A	
Self-Assembly of Small Molecules in the Cellular Milieu AMTSP				A	
Chemical Probes for Bacterial Imaging **				P	
National Fresenius Award: Symposium in Honor of Neal K. Devaraj *(ORGN)	A				
Cellulose Structure & Biosynthesis *(CELL)	D	D	A		
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges *(INOR)	P		D		
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Science for a Sustainable Energy Future *(PRES)		D			
Undergraduate Research Posters *(CHED)		P			
Rising Star Award Symposium *(WCC)		P			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer *(I&EC)		P			
ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of Yvonne C. Martin *(COMP)			D		
Chemical Biology: Enabling Drug Discovery *(ORGN)				A	

Division of Business Development & Management — BMGT

J. Bryant, Program Chair

Hotel Nikko San Francisco	S	M	Tu	W	Th
Chemical Angel Network: Chemists Investing in Chemical Companies **	P				
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
ACS Award in the Chemistry of Materials: Symposium in Honor of Douglas A. Keszler *(INOR)	E		D		
Entrepreneurial Opportunities in Chemistry *(YCC)	E				
Teaching, Researching & Community Building in the Global Chemical Enterprise *(IAC)		D			
Science for a Sustainable Energy Future *(PRES)		D			
Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators *(PROF)			A		
Looking Beyond Your Current Boundaries: What's the Next Step? *(PROF)				D	

Division of Carbohydrate Chemistry — CARB

N. Snyder, Program Chair

Grand Hyatt San Francisco	S	M	Tu	W	Th
Wolfrom Award	A				
Isbell Award	P				
Gin New Investigator Award	P				
Hudson Award		A			
Carbohydrate-Based Hybrid Materials for Nanomedicine **		P	A		
Sci-Mix		E			
LPS: Chemistry, Synthesis & Applications **			D		
General Posters			E		
Carbohydrate-Based Nanomaterials & Drug-Delivery Vehicles **				D	
Cellulose Structure & Biosynthesis *(CELL)	D	D	A		

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Division of Carbohydrate Chemistry — CARB

N. Snyder, Program Chair

Grand Hyatt San Francisco	S	M	Tu	W	Th
Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in Honor of Kevin J. Edgar *(CELL)	D	D	D		
Hollyweird Chemistry *(CPRC)	P	D			
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Functional Lignocellulosics & Nanotechnology *(CELL)		D	D	D	D
Science for a Sustainable Energy Future *(PRES)		D			
Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials *(CATL)		P	D		
Advances in Polysaccharides: Practice & Applications *(CELL)			P	D	D
Biobased Gels & Porous Materials *(CELL)				D	D
Frontiers in Glycoanalytics *(CELL)				P	A

Division of Catalysis Science & Technology — CATL

E. Nikolla, S. Scott, Program Chairs

Parc 55 San Francisco	S	M	Tu	W	Th
Amorphous Catalytic Materials AMTSP	D	A			
Advanced X-Ray Techniques for Catalyst Characterization ** AMTSP	D	D	A		
Elucidation of Mechanisms & Kinetics on Surfaces ** AMTSP	D	D	D	D	D
Electrocatalysis for Energy Generation & Storage ** AMTSP	D	D			
ACS Award in Surface Chemistry: Symposium in Honor of Cynthia M. Friend ** AMTSP	D	D			
Synthesis of Catalysts by Nontraditional Methods ** AMTSP	D				
Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis ** AMTSP		D	D	D	
Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials ** AMTSP		P	D		
Operando Methodology at the Junction Between Fundamental Chemistry & Chemical Engineering ** AMTSP			D	D	D
Designed Catalysis: Materials Genome Approach to Heterogeneous Processes ** AMTSP			D	D	D
General Papers AMTSP			P	P	P

Division of Catalysis Science & Technology — CATL

E. Nikolla, S. Scott, Program Chairs

Parc 55 San Francisco	S	M	Tu	W	Th
Poster Session AMTSP			E		
Single-Site Heterogeneous Catalysts AMTSP				D	A
Subsurface Technologies for Recovery of Fossil & Geothermal Energy *(ENFL)	A				
Catalysis for Unconventional Energy Sources *(ENFL)	D	A			
Molecular Surface Science, Nanomaterials & Catalysis: Symposium in Honor of Gabor Somorjai at 80 *(COLL)	D	D	A	D	
Synthesis & Characterization of Materials for Energy Applications *(ANYL)	D	D	D	D	
Catalytic Materials from Molecular Insight *(COMP)	D	D	D		
Advanced Materials & Technologies for Solar Energy Conversion & Storage *(ENFL)	D	D	D		
C1 Catalysis *(ENFL)	D	D			
Computations for CO_2 Capture, Conversion & Sequestration *(ENFL)	D	D			
Sustainability in Electrocatalytic Fuel & Chemical Production *(INOR)	DE	P			
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Support & Activator Effects on Metal-Mediated Polymerization *(PMSE)		D	D		
Science for a Sustainable Energy Future *(PRES)		D			
Functional Porous Materials for Sustainable Energy *(ENFL)			D	D	A
State-of-the-Art Methods for Modeling Materials Chemistry *(COMP)			D	D	
ACS Award Lectures *(COLL)			P		
13th International Symposium on Heavy Oil Upgrading, Production & Characterization *(ENFL)				D	A

Division of Cellulose & Renewable Materials — CELL

M. Roman, Program Chair

Moscone Center	S	M	Tu	W	Th
Cellulose Structure & Biosynthesis **	D	D	A		
Processing & Properties of Biobased Composites & Blends	D	D	D	A	
Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in Honor of Kevin J. Edgar **	D	D	D		
Nanocellulose Processing & Analysis **	D	D			
Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems **	D	P	D	D	D
New Horizons in Sustainable Materials **	D				
General Posters	E				
Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy ** AMTSP		A			
Functional Lignocellulosics & Nanotechnology ** AMTSP		D	D	D	D
Sci-Mix		E			
Developments in the Fields of Celluloses & Lignocelluloses: In Honor of Dr. Rajai Atalla **			D	D	D
Advances in Polysaccharides: Practice & Applications **			P	D	D
Biobased Gels & Porous Materials ** AMTSP				D	D
Frontiers in Glycoanalytics ** AMTSP				P	A
Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry ** AMTSP				P	D
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Science for a Sustainable Energy Future: Energy Storage *(PRES)		D			
Carbohydrate-Based Hybrid Materials for Nanomedicine *(CARB)		P	A		
Biomass & Biofuel Processing *(ENFL)			D	D	
LPS: Chemistry, Synthesis & Applications *(CARB)			D		
Carbohydrate-Based Nanomaterials & Drug-Delivery Vehicles *(CARB)				D	

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Division of Chemical Education — CHED

T. Miller, I. Levy, C. Muzzi, Program Chairs

San Francisco Marriott Marquis	S	M	Tu	W	Th
Eye Tracking Research in Chemistry Education	A				
Undergraduate Research Papers **	D	D			
Research in Chemistry Education	D			D	
Citizens First! **	D				
Green Chemistry: Theory & Practice **	D				
High School Program **	D				
NMR Spectroscopy in the Undergraduate Curriculum	D				
State of the Art: Applying Chemistry Education Research to Practice	D				
Celebrating Chemistry Through Outreach: Honoring the Legacy of Christine Jaworek-Lopes	P				
General Posters	E				
ACS-CEI Award for Incorporating Sustainability into Chemistry Education		A			
Chemistry Education Research: Graduate Student Research Forum		A			
Advances in e-Learning & Online Chemical Education		D	A		
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Symposium in Honor of Marcy H. Towns **		D			
Curricular Innovations in Undergraduate Chemical Education Impacted by NSF		D			
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment **		D			
International & Multicultural Perspective **		P			
Process-Oriented Guided Inquiry Learning (POGIL)		P			
Undergraduate Research Posters **		P			
Innovating Materials for the Next Generation: Bringing Practical Applications into the Chemistry Classroom ** AMTSP		E			
Successful Student Chapters **		E			
Sci-Mix		E			
Perspectives on Climate Change Literacy & Education: Local to International **			A		
ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in Honor of Saundra Y. McGuire **			A		
Advancing Undergraduate Research ** AMTSP			D	A	
Advances in Teaching Organic Chemistry			D		
George C. Pimentel Award in Chemical Education: Symposium to Honor Thomas A. Holme			D		
GSSPC: Water Sustainability **			D		
Course-Based Undergraduate Research Experiences (CUREs) in Chemistry			P	D	

Division of Chemical Education CHED

T. Miller, I. Levy, C. Muzzi, Program Chairs

San Francisco Marriott Marquis	S	M	Tu	W	Th
Simulations, Animations & Other Visualizations in Educating about Chemistry Save Chemistry!			P		
The Role of Research Experiences in the ACS Certified Degree			P		
Writing in Chemistry			P		
Research on Learning in the Lab **				A	
Communicating Science in the 21st Century to Diversified Audiences **				D	
Strategies Promoting Success of Two-Year College Students				D	
Undergraduate Laboratory Experiments Involving Advanced Materials **				D	
Using Chemistry Education Research to Inform the Design & Use of Assessment Materials				D	
General Papers				P	A
Eliciting Attentiveness from Cyber-Savvy Students Without Using Electronic Tools				P	
How Do We Teach Collaboration? Best Practices for Educating Future Researchers & Innovators **					A
Instructors & Researchers: Advancing Graduate Student Education					A
The General Chemistry Course for a Changing World					A
Engaging Students in Physical Chemistry **					A
Current Best Practices for Chemistry REU Programs **					A
Undergraduate Symposium *(AGFD)	A				
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Incorporating Polymer Science into the Classroom *(POLY)	D				
Blending Chemistry & Culture: Undergraduate Research Abroad Through ACS IREU Program *(IAC)	D				
Textbooks & the Practice of Science: Before, During & After Gutenberg *(CINF)	P	D			
Hollyweird Chemistry *(CPRC)	P	D			
The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross *(WCC)	P		A		
Withycombe–Charalambous Graduate Student Symposium *(AGFD)	P				
Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences *(ENVR)		P		E	
The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit *(CINF)		P			

Division of Chemical Education CHED

T. Miller, I. Levy, C. Muzzi, Program Chairs

San Francisco Marriott Marquis	S	M	Tu	W	Th
Processes, Technologies & Sensors for Food-Energy-Water Nexus Research *(ENVR)			A		
Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators *(PROF)			A		
Science & Perception of Climate Change *(ENVR)			P	E	
Active Learning in the Undergraduate Analytical Chemistry Curriculum *(ANYL)				D	
How Do We Teach Collaboration? Best Practices for Educating Future Researchers & Innovators *(CHED)					A

Division of Chemical Health & Safety CHAS

D. Decker, J. Pickel, F. Wood-Black, Program Chairs

Park Central San Francisco	S	M	Tu	W	Th
Ask Dr. Safety: Chemical & Occupational Safety in the Cannabis Industry **	P				
Best Practices in Selecting & Presenting Safety Training Content **	P				
Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing **		D			
Sci-Mix		E			
Information Flow in Environmental Health & Safety **			D		
What Have We Learned & Where Are We Going: Post-Settlement in the University of California **				D	
Nanocellulose Processing & Analysis *(CELL)	D	D			
Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce *(CHAL)			P		
Cannabis: A Growing Sector for Business & Employment *(SCHB)				A	

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E = EVE DE = AM/PM/EVE PE = PM/EVE

Division of Chemical Information — CINF

E. Alvaro, Program Chair

Park Central San Francisco	S	M	Tu	W	Th
Careers in Chemical Information	A				
Open Access: Current Landscape, Challenges & Future Directions	D		D		
Materials Informatics & Computational Modeling ** AMTSP	D				
Textbooks & the Practice of Science: Before, During & After Gutenberg **	P	D			
CINF Scholarships for Scientific Excellence: Student Poster Competition	E				
Advances in Data Visualization		A			
Advances in High-Throughput Screening **		D			
The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit **		P			
Sci-Mix		E			
Advanced Materials: Issues in Nanoinformatics & Nanosafety Data AMTSP			A		
Text-Mining & Natural Language Processing for Chemical Information: From Documents to Knowledge			D		
Assessment of Chemistry Collections & Services				A	
General Papers				D	
Public-Private Partnerships: Fostering Drug Discovery & Data Sharing **				D	
Should I Move My Computational Chemistry or Informatics Tools to the Cloud? *(COMP)	D	D			
Computer-Aided Peptide Design *(COMP)	D				
Data Science Challenges in Computational Chemistry *(COMP)		P			
Information Flow in Environmental Health & Safety *(CHAS)			D		

Division of Chemistry & the Law — CHAL

K. Bianco, J. Kennedy, Program Chairs

Park Central San Francisco	S	M	Tu	W	Th
Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions	P				
Patent Challenges & Chocolate: A Sweet & Sour Symposium		A			
Nontraditional Careers in Chemistry		A			
The Use of Scientific Information in IP-Related Matters		P			
Sci-Mix		E			
An International Perspective: Patent Eligible Subject Matter & Opposition Procedures			A		
Protecting & Capitalizing on Your Intellectual Property			P		
Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce **			P		

Division of Chemistry & the Law — CHAL

K. Bianco, J. Kennedy, Program Chairs

Park Central San Francisco	S	M	Tu	W	Th
Cannabis Law: Navigating Complex Regulatory & Legal Issues in States with Legal Cannabis Programs				A	
The Many Faces of CHAL: Where Chemistry Meets the Law				P	
A Decade of U.S. Supreme Court Patent Jurisprudence				P	
Chemical Forensics *(ANYL)		D	D		

Division of Colloid & Surface Chemistry — COLL

R. Nagarajan, Program Chair

Moscone Center	S	M	Tu	W	Th
Basic Research in Colloids, Surfactants & Nanomaterials	AE			D	A
Applied Biosensing Based on Functional Colloids AMTSP	D	D	A	A	
Biomembrane Synthesis, Structure, Mechanics & Dynamics	D	D	A	D	A
Molecular Surface Science, Nanomaterials & Catalysis: Symposium in Honor of Gabor Somorjai at 80 **	D	D	A	D	
Coacervation: Physics, Chemistry & Biology AMTSP	D	D			
Chemistry & Physics of Tribology AMTSP	D		A	D	
Colloidal Nanoparticle Synthesis & Assembly	DE	D	A	D	A
Interfacial Phenomena & the Oil-Water Interface AMTSP	DE	D			
Nanoscale Chemical Patterning & Characterization	DE	D			
Deposition & Etching of Nanostructures ** AMTSP	DE		D		
Nanostructure Engineering & Surface Chemistry for Spectroscopy, Imaging & Alternative Energy Harvesting & Conversion AMTSP	P	D	A		
Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment	E	D	A	D	A
Fundamental Research in Colloids, Surfaces & Nanomaterials	E				
ACS Award in Colloid Chemistry: Symposium in Honor of Nicholas A. Kotov		D	A		
Sci-Mix		E			
ACS Award for Research at an Undergraduate Institution: Symposium in Honor of Maria Hepel			A		
ACS Award Lectures **			P		
Mineral-Water Interface Chemistry *(GEOC)	D	A	D	AE	

Division of Colloid & Surface Chemistry — COLL

R. Nagarajan, Program Chair

Moscone Center	S	M	Tu	W	Th
Elucidation of Mechanisms & Kinetics on Surfaces *(CATL)	D	D	D	D	D
Janus Particles: Synthesis, Characterization & Applications *(PMSE)	D	D			
ACS Award in Surface Chemistry: Symposium in Honor of Cynthia M. Friend *(CATL)	D	D			
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Separation of Macromolecules & Particulates *(POLY)	D				
Synthesis of Catalysts by Nontraditional Methods *(CATL)	D				
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Functional Lignocellulosics & Nanotechnology *(CELL)		D	D	D	D
Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis *(CATL)		D	D	D	
Science for a Sustainable Energy Future *(PRES)		D			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer *(I&EC)		P			
Chemical Principles of Environmental, Cellular & Organismal Nanotoxicology *(ENVR)				AE	
Biobased Gels & Porous Materials *(CELL)				D	D
Deposition & Etching of Nanostructures *(INOR)				D	
Evolving Nanoparticle Reactivity Throughout Nucleation, Growth & Dissolution *(GEOC)				D	

Division of Computers in Chemistry — COMP

H. Woodcock, M. Feig, J. Shen, Program Chairs

InterContinental San Francisco	S	M	Tu	W	Th
Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling **	A	D	A	D	D
Computational Studies of Water	D	A			
Catalytic Materials from Molecular Insight ** AMTSP	D	D	D		
Strong Electron Correlation & Nonadiabatic Dynamics **	D	D	D		
Should I Move My Computational Chemistry or Informatics Tools to the Cloud? **	D	D			
Computer-Aided Peptide Design **	D				

Division of Computers in Chemistry — COMP

H. Woodcock, M. Feig, J. Shen, Program Chairs

InterContinental San Francisco	S	M	Tu	W	Th
Undergraduate Research & National Meeting Roundtable	P				
Drug Design		D		D	D
Data Science Challenges in Computational Chemistry **		P			
Sci-Mix		E			
Molecular Mechanics			A	D	D
State-of-the-Art Methods for Modeling Materials Chemistry **			D	D	
ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of Yvonne C. Martin **			D		
Material Science			P	D	D
Quantum Mechanics			P	D	D
Chemical Computing Group Graduate Student Travel Awards			E		
COMP Poster Session			E		
NVIDIA GPU Award			E		
OpenEye Outstanding Junior Faculty Award			E		
Wiley Computers in Chemistry Outstanding Postdoc Award			E		
Quantum Dynamics in Large-Scale Systems *(PHYS)	D	D	D		
Computations for CO_2 Capture, Conversion & Sequestration *(ENFL)	D	D			
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Materials Informatics & Computational Modeling *(CINF)	D				
Advances in High-Throughput Screening *(CINF)		D			
Undergraduate Research Posters *(CHED)		P			
Designed Catalysis: Materials Genome Approach to Heterogeneous Processes *(CATL)			D	D	D
Public-Private Partnerships: Fostering Drug Discovery & Data Sharing *(CINF)				D	

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Division of Energy & Fuels — ENFL

D. Heldebrant, Program Chair

Grand Hyatt San Francisco	S	M	Tu	W	Th
Subsurface Technologies for Recovery of Fossil & Geothermal Energy ** AMTSP	A				
Catalysis for Unconventional Energy Sources ** AMTSP	D	A			
Advanced Materials & Technologies for Solar Energy Conversion & Storage **	D	D	D		
C1 Catalysis **	D	D			
Computations for CO_2 Capture, Conversion & Sequestration ** AMTSP	D	D			
Advanced Analytical Techniques for Determination of Minor & Trace Elements in Petroleum Value Chain AMTSP	D				
Innovative Chemistry & Materials for Electrochemical Energy Storage ** AMTSP	P	D	D	D	A
Advances in Chemistry of Energy & Fuels AMTSP		D	D	D	A
ENFL Distinguished Researcher Award: Symposium in Honor of Mieczyslaw M. Boduszynski		P			
Sci-Mix		E			
Functional Porous Materials for Sustainable Energy ** AMTSP			D	D	A
Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies ** AMTSP			D	D	
Biomass & Biofuel Processing **			D	D	
13th International Symposium on Heavy Oil Upgrading, Production & Characterization **				D	A
Cellulose Structure & Biosynthesis *(CELL)	D	D	A		
Electrocatalysis for Energy Generation & Storage *(CATL)	D	D			
Hollyweird Chemistry *(CPRC)	P	D			
Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy *(CELL)		A			
Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis *(CATL)		D	D	D	
Science for a Sustainable Energy Future *(PRES)		D			
Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials *(CATL)		P	D		
Rising Star Award Symposium *(WCC)		P			

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Division of Environmental Chemistry — ENVR

S. Obare, S. Al-Abed, Program Chairs

San Francisco Marriott Marquis (Thursday only: Moscone Center)	S	M	Tu	W	Th
Have Great Lakes Restoration Programs Been Successful? The Case of Legacy & Emerging Pollutants	A			E	
Accurate Mass/High-Resolution Mass Spectrometry for Environmental Monitoring & Remediation ** AMTSP	D	A		E	
Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in Honor of Prof. Jun Ma AMTSP	D	D	D	A	
Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse AMTSP	D	D	D	DE	
Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium Honoring the Contributions of Mel Suffet	D	D	D	E	
Understanding Dissolved Organic Matter Reactivity: Honoring George Aiken, the DOM Whisperer	D	D	D		
Contaminants of Emerging Concern in Natural & Engineered Systems ** AMTSP	D	D		E	
Tribute to Jerry Schnoor	D	D			
Green Chemistry & the Environment **	D			E	
Integrated & Sustainable Environmental Remediation **	P			E	
Advances & Applications in Water Sensing Technologies for Drinking Water, Re-Use, Agri-Tech & Research		A		E	
Sulfidation of Metal-Based Engineered & Natural Nanomaterials: Implications for Their Fate & Effects in the Environment AMTSP		D		E	
Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences **		P		E	
Nanomaterials in Consumer Products: Formulation, Characterization & Applications Across the Product Life Cycle		P		E	
Sci-Mix		E			
Processes, Technologies & Sensors for Food-Energy-Water Nexus Research ** AMTSP			A		
Innovative Materials & Technologies for Sustainable Water Purification ** AMTSP			D	DE	D

Division of Environmental Chemistry — ENVR

S. Obare, S. Al-Abed, Program Chairs

San Francisco Marriott Marquis (Thursday only: Moscone Center)	S	M	Tu	W	Th
From the Bench to the Field: Evaluating Innovative Remediation & Detection Technologies			D	E	
ACS Award for Creative Advances in Environmental Science & Technology: Symposium in Honor of Dr. Douglas R. Worsnop AMTSP			D		
Green Chemistry Adoption: Progressive Changes by Different Industry Sectors **			D		
Science & Perception of Climate Change **			P	E	
Great Achievements in Environmental Science & Technology: James J. Morgan Award Symposium				A	
Chemical Principles of Environmental, Cellular & Organismal Nanotoxicology **				AE	
Whole Organism Metrology to Support Nanotoxicology Research in the Environment				D	
Poly- & Per-Fluoroalkyl Substances: Where, What, When, Why, Who & How AMTSP				DE	A
Aquatic Photochemistry **				DE	D
Novel Membrane Materials & Processes for Water Purification AMTSP				DE	D
Advances in Resource Recovery & Conservation in Water Systems ** AMTSP				PE	D
Contaminants in Urban & Coastal Estuarine Ecosystems ** AMTSP				PE	D
Pesticides in Surface Water: Monitoring, Modeling, Mitigation, Risk Assessment & Regulation				PE	D
Applications of Cheminformatics & Computational Chemistry in Environmental Health				E	D
Bioprocesses for Engineered Nanomaterials in Soil-Plant Systems AMTSP				E	D
Clay Minerals Selectivity & Its Environmental Applications				E	
New Challenges in Environmental Chemistry: Marine Ecosystems & Microplastics				E	
General Posters				E	
Mineral-Water Interface Chemistry *(GEOC)	D	A	D	AE	
Elucidation of Mechanisms & Kinetics on Surfaces *(CATL)	D	D	D	D	D

Division of Environmental Chemistry — ENVR

S. Obare, S. Al-Abed, Program Chairs

San Francisco Marriott Marquis (Thursday only: Moscone Center)	S	M	Tu	W	Th
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Advances in Treatment Processes for Metals & Metalloids *(GEOC)		A		E	
Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy *(CELL)		A			
Teaching, Researching & Community Building in the Global Chemical Enterprise *(IAC)		D			
Science for a Sustainable Energy Future *(PRES)		D			
Undergraduate Research Posters *(CHED)		P			
Operando Methodology at the Junction Between Fundamental Chemistry & Chemical Engineering *(CATL)			D	D	D
Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce *(CHAL)			P		
Evolving Nanoparticle Reactivity Throughout Nucleation, Growth & Dissolution *(GEOC)				D	
Environmental Challenges & Solutions in Unconventional Oil & Gas Development *(GEOC)				E	D
Contaminants Transport, Uptake & Remediation at Contaminated Sites *(GEOC)				E	D

Division of Fluorine Chemistry — FLUO

N. Vasdev, Program Chair

Grand Hyatt San Francisco	S	M	Tu	W	Th
ACS Award for Creative Work in Fluorine Chemistry: Symposium in Honor of Antonio Togni	DE	D	D		
Sci-Mix		E			
General Papers			P		
General Posters			E		

Division of Geochemistry — GEOC

A. Ilgen, Program Chair

San Francisco Marriott Union Square	S	M	Tu	W	Th
Mineral-Water Interface Chemistry **	D	A	D	AE	
Redox-Driven Environmental Geochemical Reactions for Metals, Major Elements & Organic Pollutants	D	A	D	E	
Pore-Scale Geochemical Processes & the Implications for CO_2 Geologic Storage	D				
Structure, Properties & Applications of Minerals with Layered Structure	D				
Advances in Treatment Processes for Metals & Metalloids **		A		E	
Formation, Structure & Reactivity of Biogenic Minerals		A		E	
2017 Geochemistry Division Medal Symposium		P			
Sci-Mix		E			
2017 Geochemistry Division Medal: Symposium in Honor of Dr. Susan Brantley			D	AE	
Microbially Driven Geochemical Reactions: Kinetics & Communities			D	DE	
Evolving Nanoparticle Reactivity Throughout Nucleation, Growth & Dissolution **				D	
Structure & Reactivity of Cementitious Materials from Advanced Characterization Techniques				PE	A
General Geochemistry				PE	
Environmental Challenges & Solutions in Unconventional Oil & Gas Development **				E	D
Contaminants Transport, Uptake & Remediation at Contaminated Sites **				E	D
Mineral Nucleation: Transient Intermediates & Phase Transitions				E	D
Subsurface Technologies for Recovery of Fossil & Geothermal Energy *(ENFL)	A				
Computations for CO_2 Capture, Conversion & Sequestration *(ENFL)	D	D			
Science for a Sustainable Energy Future *(PRES)		D			
Undergraduate Research Posters *(CHED)		P			
Aquatic Photochemistry *(ENVR)				DE	D
Advances in Resource Recovery & Conservation in Water Systems *(ENVR)				PE	D

Division of the History of Chemistry — HIST

S. Rasmussen, Program Chair

Grand Hyatt San Francisco	S	M	Tu	W	Th
General Papers	A			A	
Golden Age of Industrial Chemistry **	P				
Chemistry Through the Eyes of Non-Chemists: Evolution of the Public Perception of Chemistry		D	A		
Sci-Mix		E			
Chemistry & the Design of Physical Objects: Innovation from 1950 to the Present AMTSP			P		
Textbooks & the Practice of Science: Before, During & After Gutenberg *(CINF)	P	D			
Hollyweird Chemistry *(CPRC)	P	D			
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				

Division of Industrial & Engineering Chemistry — I&EC

E. Rosenberg, Program Chair

Grand Hyatt San Francisco	S	M	Tu	W	Th
I&EC International Fellow Symposium: Honoring Prof. Kew-Ho Lee	A				
Ionic Liquids in Separations & Analysis	P				
I&EC Division Fellow Award Symposium: Honoring Prof. Klavs Jensen	P				
2017 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Gregg Beckham		A			
Symposium in Honor of Michelle Cummings, ACT Fellow AMTSP		A			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer ** AMTSP		P			
2017 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Jinlong Gong		P			
Sci-Mix		E			
2017 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in Honor of Helen Sneddon			A		
2016 E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Michael M. Thackeray			D		
I&EC Division Early Career Fellow Symposium: Honoring Dr. Leigh Martin				D	
General Posters				E	
General Papers					D

Division of Industrial & Engineering Chemistry — I & E C

E. Rosenberg, Program Chair

Grand Hyatt San Francisco	S	M	Tu	W	Th
Nanocellulose Processing & Analysis *(CELL)	D	D			
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis *(CATL)		D	D	D	
Teaching, Researching & Community Building in the Global Chemical Enterprise *(IAC)		D			
Science for a Sustainable Energy Future *(PRES)		D			
Operando Methodology at the Junction Between Fundamental Chemistry & Chemical Engineering *(CATL)			D	D	D
Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce *(CHAL)			P		
2017 E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in Honor of Eleftherios T. Papoutsakis *(BIOT)				A	

Division of Inorganic Chemistry — I N O R

S. Koch, N. Radu, Program Chairs

Moscone Center	S	M	Tu	W	Th
Lanthanide & Actinide Chemistry **	A		E	A	D
Bioinorganic Chemistry	A		PE	A	A
Organometallic Chemistry	AE	P	PE	D	D
Coordination Chemistry	AE		E	P	D
Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions	D	P	AE		
Chemistry of Materials	D		DE	D	D
Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in Honor of Nilay Hazari	D				
Undergraduate Research at the Frontiers of Inorganic Chemistry	DE	P	A		
Celebrating 60 Years of the Division of Inorganic Chemistry	DE	P	D	D	
Sustainability in Electrocatalytic Fuel & Chemical Production **	DE	P			
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Pingyun Feng	DE	P			

Division of Inorganic Chemistry — I N O R

S. Koch, N. Radu, Program Chairs

Moscone Center	S	M	Tu	W	Th
ACS Award in Inorganic Chemistry: Symposium in Honor of Lawrence Que Jr.	DE				
2017 Priestley Medalist: Symposium in Honor of Tobin J. Marks **	P	P	D	D	
ACS Award in Organometallic Chemistry: Symposium in Honor of Marcetta Y. Darensbourg	P	P			
Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges **	P		D		
Inorganic Catalysts	P		E		D
Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in Honor of John E. Bercaw	E	P	A		
Switchable Catalysts	E	P	D	A	
ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in Honor of William B. Tolman	E		D		
ACS Award in the Chemistry of Materials: Symposium in Honor of Douglas A. Keszler ** AMTSP	E		D		
Nanoscience	E			A	P
ACS Awards in Inorganic Chemistry: Plenary Session		A			
ACS Awards: Symposium in Honor of Lawrence Que Jr. & William B. Tolman		P			
Sci-Mix		E			
Chemistry Is Central to Applied Materials **			AE	A	
Emergent Phenomena in the Solid State			DE		
Solid-State Inorganic Chemistry			E	A	A
Main Group Chemistry			E	P	P
Environmental & Energy-Related Inorganic Chemistry			E	P	
Inorganic Spectroscopy			E	P	
Electrochemistry			E		A
Deposition & Etching of Nanostructures **				D	
Frontiers in Heavy Element Electronic Structure **				D	
Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory *(PHYS)	D	D	D	D	
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Synthesis of Catalysts by Nontraditional Methods *(CATL)	D				
Deposition & Etching of Nanostructures *(COLL)	DE		D		
Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of David L. Clark *(NUCL)	P	D	D		

Division of Inorganic Chemistry INOR

S. Koch, N. Radu, Program Chairs

Moscone Center	S	M	Tu	W	Th
Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis *(CATL)		D	D	D	
Support & Activator Effects on Metal-Mediated Polymerization *(PMSE)		D	D		
Undergraduate Research Posters *(CHED)		P			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer *(I&EC)		P			
Metalloprotein-Initiated Signaling Transduction Response to Redox Stress *(BIOL)			A		
Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten *(NUCL)			D		

Division of Medicinal Chemistry MEDI

A. Stamford, Program Chair

Moscone Center	S	M	Tu	W	Th
Macrocycles & Cyclopeptides in Medicinal Chemistry	A				
General Orals	D		P	P	
Medicinal Chemists' Toolbox: Factors Influencing Oral Bioavailability & Case Studies	P				
General Posters	E			E	
Actually, It Does Work: Success with Allosteric Kinase Ligands & Phosphatase Modulators		A			
Residence Time: Not Just Affinity for Drug Design		A			
Kinase Inhibitors for Immuno-Inflammatory Diseases		P			
Misfolded Proteins in Neurodegenerative Diseases		P			
Sci-Mix		E			
Antibiotic Drug Discovery: The Next Frontier			A		
MEDI Awards Symposium			A		
Drug Discovery for ALS: Putting the Ice Bucket to Work			P		
Targeting Epigenetic Writers & Erasers				A	
First-Time Disclosures				D	
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				

Division of Medicinal Chemistry MEDI

A. Stamford, Program Chair

Moscone Center	S	M	Tu	W	Th
Advances in High-Throughput Screening *(CINF)		D			
Science for a Sustainable Energy Future: Energy Storage *(PRES)		D			
Undergraduate Research Posters *(CHED)		P			
Eminent Scientist Lecture with Dr. Carolyn Bertozzi *(SOCED)		P			
ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of Yvonne C. Martin *(COMP)			D		
Green Chemistry Adoption: Progressive Changes by Different Industry Sectors *(ENVR)			D		
Entrepreneurship in Biotechnology, Advanced Materials, Drug Discovery & Information Systems *(SCHB)			P		

Division of Nuclear Chemistry & Technology NUCL

A. Hixon, Program Chair

Moscone Center	S	M	Tu	W	Th
Nuclear Fission	D				
Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in Honor of David L. Clark **	P	D	D		
Nuclear & Radiochemistry Summer School: Past, Present & Future		D			
Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten **			D		
Advanced Actinide Materials: Nanostructure, Complexity & Extreme Environments AMTSP				D	
General Topics in Nuclear Chemistry & Technology				DE	A
Young Investigators in Nuclear & Radiochemistry **					D
Hollyweird Chemistry *(CPRC)	P	D			
Evolving Nanoparticle Reactivity Throughout Nucleation, Growth & Dissolution *(GEOC)				D	
Frontiers in Heavy Element Electronic Structure *(INOR)				D	

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Division of Organic Chemistry ORGN

R. Broene, S. Silverman, Program Chairs

Moscone Center	S	M	Tu	W	Th
National Fresenius Award: Symposium in Honor of Neal K. Devaraj **	A				
George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in Honor of Robert H. Grubbs	A				
Biologically Related Molecules & Processes	D	D	E		
Metal-Mediated Reactions & Syntheses	DE	D	A		
New Reactions & Methodology	DE	D	D	D	A
Asymmetric Reactions & Syntheses	DE	D			
Herbert C. Brown Award for Creative Research in Synthetic Methods: Symposium in Honor of Bruce H. Lipshutz	P				
Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in Honor of Neil K. Garg		A			
Computer-Guided Organic Synthesis		A			
Ernest Guenther Award in the Chemistry of Natural Products: Symposium in Honor of Stephen F. Martin		P			
Application of Physical Organic Chemistry to Challenges in Industry		P			
Sci-Mix		E			
ACS Award for Creative Work in Synthetic Organic Chemistry: Symposium in Honor of Matthew S. Sigman			A		
Heterocycles & Aromatics			D	DE	
Advances in Organic Synthesis: Successes from Academia-Industry Partnerships			D		
Molecular Recognition & Self-Assembly			DE	A	
Total Synthesis of Complex Molecules			P	DE	A
James Flack Norris Award in Physical Organic Chemistry: Symposium in Honor of Robert A. Moss			P		
Materials, Devices & Switches AMTSP			E	P	A
Peptides, Proteins & Amino Acids			E	P	
Advanced Materials Technologies, Systems & Processes AMTSP			E		P
Chemistry of Fullerenes, Carbon Nanotubes & Graphene			E		
Nanomaterials			E		
Chemical Biology: Enabling Drug Discovery **				A	
Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in Honor of Junqi Li & Martin D. Burke **				A	
Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species				PE	D
Flow Chemistry & Continuous Processes				E	A

Division of Organic Chemistry ORGN

R. Broene, S. Silverman, Program Chairs

Moscone Center	S	M	Tu	W	Th
Chemistry of Nanomaterials, Fullerenes, Carbon Nanotubes & Graphene					A
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
Science for a Sustainable Energy Future *(PRES)		D			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer *(I&EC)		P			
Green Chemistry Adoption: Progressive Changes by Different Industry Sectors *(ENVR)			D		

Division of Physical Chemistry PHYS

J. Shea, Program Chair

Parc 55 San Francisco	S	M	Tu	W	Th
Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities	D	A	P	D	A
Long-Range Correlated Motions in Proteins	D	D	A		
PHYS Division Awards Symposium	D	D	D	A	
Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi	D	D	D	D	
Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory ** AMTSP	D	D	D	D	
Quantum Dynamics in Large-Scale Systems ** AMTSP	D	D	D		
Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains		D	D	D	A
Spectroscopy of Complex Systems AMTSP		P	D	D	A
Sci-Mix		E			
Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts AMTSP				D	D
PHYS Poster Session				E	
Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling *(COMP)	A	D	A	D	D
Advanced X-Ray Techniques for Catalyst Characterization *(CATL)	D	D	A		

Division of Physical Chemistry PHYS

J. Shea, Program Chair

Parc 55 San Francisco	S	M	Tu	W	Th
Synthesis & Characterization of Materials for Energy Applications *(ANYL)	D	D	D	D	
Catalytic Materials from Molecular Insight *(COMP)	D	D	D		
Strong Electron Correlation & Nonadiabatic Dynamics *(COMP)	D	D	D		
Coherent Multidimensional Spectroscopy in Materials Science *(ANYL)	D	D			
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Engaging Students in Physical Chemistry *(CHED)					A

Division of Polymer Chemistry POLY

C. Lipscomb, T. White, T. Epps, Program Chairs

Moscone Center	S	M	Tu	W	Th
Next Generation Smart Materials ** AMTSP	A	D	D	D	A
General Topics: New Synthesis & Characterization of Polymers	D	A	DE	D	A
Contributions of IBM Almaden to Polymer Science ** AMTSP	D	A			
Polymeric Materials for Performance & Sustainability **	D	D	AE	D	A
Polymer Applications & Characterization in the Biomedical Industry AMTSP	D		E		
Incorporating Polymer Science into the Classroom **	D				
Separation of Macromolecules & Particulates ** AMTSP	D				
Carl S. Marvel Creative Polymer Chemistry Award in Honor of Theresa M. Reineke	P				
Excellence in Graduate Polymer Research ** AMTSP		D	DE		
Undergraduate Research in Polymer Science		D	E		
50th Anniversary Celebration of Macromolecules ** AMTSP		D			
Industrial Innovations in Polymer Chemistry **		P			
Sci-Mix		E			
Polymer Chemistry (RSC) Lectureship **			D		
Structure to Function in Supramolecular Polymers & Materials AMTSP			DE	D	A
Polymers & Biomimicry AMTSP			P	D	A
Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications ** AMTSP			E	D	A
ACS Award in Polymer Chemistry: Symposium in Honor of Murugappan Muthukumar **				P	

Division of Polymer Chemistry POLY

C. Lipscomb, T. White, T. Epps, Program Chairs

Moscone Center	S	M	Tu	W	Th
POLY/PMSE Plenary Lecture & Awards **				E	
Frontiers in Nanoscience *(SOCED)	A				
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Materials Informatics & Computational Modeling *(CINF)	D				
New Horizons in Sustainable Materials *(CELL)	D				
Hollyweird Chemistry *(CPRC)	P	D			
Undergraduate Research Posters *(CHED)		P			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer *(I&EC)		P			
Innovating Materials for the Next Generation: Bringing Practical Applications into the Chemistry Classroom *(CHED)		E			
Developments in the Fields of Celluloses & Lignocelluloses: In Honor of Dr. Rajai Atalla *(CELL)			D	D	D
Polymers Under Deformation *(PMSE)			D	D	
Recent Advances in Multiblock Copolymers *(PMSE)			P	D	A
Advances in Polysaccharides: Practice & Applications *(CELL)			P	D	D
Biobased Gels & Porous Materials *(CELL)				D	D
Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry *(CELL)				P	D

Division of Polymeric Materials Science & Engineering PMSE

A. Tsou, M. Grunlan, B. Olsen, X. Jia, C. Snyder, Program Chairs

Moscone Center	S	M	Tu	W	Th
Nanoscale Spectroscopic Characterization of Catalysts & Polymers AMTSP	D	D			
Young Investigators Symposium ** AMTSP	D	D			
Janus Particles: Synthesis, Characterization & Applications ** AMTSP	D	D			
ACS Award in Applied Polymer Science: Symposium in Honor of Zhenan Bao ** AMTSP	D	D			
General Papers/New Concepts in Polymeric Materials AMTSP	D		D	D	D
1D Nanomaterials: Synthesis, Assembly, Properties & Applications AMTSP	D				
Molecular Engineering of Peptide Assembly AMTSP		D	D	D	
Synthesis, Processing & Device Engineering of Polymeric Electronic Materials AMTSP		D	D	D	
Support & Activator Effects on Metal-Mediated Polymerization ** AMTSP		D	D		

Division of Polymeric Materials Science & Engineering — PMSE

A. Tsou, M. Grunlan, B. Olsen, X. Jia, C. Snyder, Program Chairs

Moscone Center	S	M	Tu	W	Th
Sci-Mix AMTSP		E			
Cooperative Research Award: Symposium in Honor of Paul A. Kohl & Edmund Elce AMTSP			A		
Biomaterials for Immunotherapy AMTSP			D	D	A
Innovations in Drug Delivery Systems & Combination Products AMTSP			D	D	
Polymers Under Deformation ** AMTSP			D	D	
Recent Advances in Multiblock Copolymers ** AMTSP			P	D	A
Joint PMSE/POLY Poster Session AMTSP			E		
Contributions of IBM Almaden to Polymer Science *(POLY) AMTSP	D	A			
Advanced Materials & Technologies for Solar Energy Conversion & Storage *(ENFL)	D	D	D		
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium *(PROF)	D	D			
Incorporating Polymer Science into the Classroom *(POLY)	D				
Separation of Macromolecules & Particulates *(POLY)	D				
Innovative Chemistry & Materials for Electrochemical Energy Storage *(ENFL)	P	D	D	D	A
2017 Priestley Medalist: Symposium in Honor of Tobin J. Marks *(INOR)	P	P	D	D	
50th Anniversary Celebration of Macromolecules *(POLY)		D			
Industrial Innovations in Polymer Chemistry *(POLY)		P			
Undergraduate Research Posters *(CHED)		P			
ACS Award in Industrial Chemistry: Symposium in Honor of Jane Frommer *(I&EC)		P			
Innovating Materials for the Next Generation: Bringing Practical Applications into the Chemistry Classroom *(CHED)		E			
Advances in Polysaccharides: Practice & Applications *(CELL)			P	D	D
Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications *(POLY)			E	D	A
Biobased Gels & Porous Materials *(CELL)				D	D
ACS Award in Polymer Chemistry: Symposium in Honor of Murugappan Muthukumar *(POLY)				P	
POLY/PMSE Plenary Lecture & Awards *(POLY)				E	

Division of Professional Relations — PROF

R. D. Libby, Program Chair

Hotel Nikko San Francisco	S	M	Tu	W	Th
LGBT Graduate & Postdoctoral Student Chemistry Research Symposium **	D	D			
General Posters	E				
Sci-Mix		E			
Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators **			A		
REU Chemistry in Action: Student Perspectives			P		
Looking Beyond Your Current Boundaries: What's the Next Step? **				D	
The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross *(WCC)	P		A		
Starting a Successful Research Program at a PUI *(YCC)	P				
Chemical Angel Network: Chemists Investing in Chemical Companies *(BMGT)	P				
Holy Grails in Chemistry: Celebrating the 50th Anniversary of *Accounts of Chemical Research* Journal *(PRES)	PE				
ACS Award in the Chemistry of Materials: Symposium in Honor of Douglas A. Keszler *(INOR)	E		D		
Entrepreneurial Opportunities in Chemistry *(YCC)	E				
Celebrating 90 years of the WCC: Reflections of Past Chairs *(WCC)		A			
Excellence in Graduate Polymer Research *(POLY)		D	DE		
Teaching, Researching & Community Building in the Global Chemical Enterprise *(IAC)		D			
Science for a Sustainable Energy Future *(PRES)		D			
Space Chemistry: How It Helps Space Exploration *(YCC)		D			
Rising Star Award Symposium *(WCC)		P			
Chemists & Writing for Fun & Profit: Write Your Own Career *(SCHB)			A		
Advancing Undergraduate Research *(CHED)			D	A	
Entrepreneurship in Biotechnology, Advanced Materials, Drug Discovery & Information Systems *(SCHB)			P		

Division of Small Chemical Businesses — SCHB

J. Sabol, Program Chair

Hotel Nikko San Francisco	S	M	Tu	W	Th
Entrepreneurs' Poster Session	A				
Sci-Mix		E			
Chemists & Writing for Fun & Profit: Write Your Own Career **			A		
Entrepreneurship in Biotechnology, Advanced Materials, Drug Discovery & Information Systems ** AMTSP			P		
Cannabis: A Growing Sector for Business & Employment **				A	
Hollyweird Chemistry *(CPRC)	P	D			
Chemical Angel Network: Chemists Investing in Chemical Companies *(BMGT)	P				
Entrepreneurial Opportunities in Chemistry *(YCC)	E				
Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing *(CHAS)		D			
Green Chemistry Adoption: Progressive Changes by Different Industry Sectors *(ENVR)			D		

Committee on Chemical Safety — CCS

E. Howson, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Ask Dr. Safety: Chemical & Occupational Safety in the Cannabis Industry *(CHAS)	P				
Best Practices in Selecting & Presenting Safety Training Content *(CHAS)	P				
Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing *(CHAS)		D			
Information Flow in Environmental Health & Safety *(CHAS)			D		
What Have We Learned & Where Are We Going: Post-Settlement in the University of California *(CHAS)				D	

Committee on Chemistry and Public Affairs — CCPA

S. Butts, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Hollyweird Chemistry *(CPRC)	P	D			

Committee on Chemists with Disabilities — CWD

J. Johnston, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Communicating Science in the Twenty-First Century to Diversified Audiences *(CHED)				D	

Committee on Community Activities — CCA

M. McGinnis, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)		D			

Committee on Divisional Activities — DAC

R. Bennett, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Young Investigators Symposium *(PMSE)	D	D			

Committee on Environmental Improvement — CEI

C. Middlecamp, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Contaminants of Emerging Concern in Natural & Engineered Systems *(ENVR)	D	D		E	
Green Chemistry & the Environment *(ENVR)	D			E	
Citizens First! *(CHED)	D				
Green Chemistry: Theory & Practice *(CHED)	D				
Hollyweird Chemistry *(CPRC)	P	D			
Integrated & Sustainable Environmental Remediation *(ENVR)	P			E	
Science for a Sustainable Energy Future *(PRES)		D			
Undergraduate Research Posters *(CHED)		P			
Processes, Technologies & Sensors for Food-Energy-Water Nexus Research *(ENVR)			A		
Perspectives on Climate Change Literacy & Education: Local to International *(CHED)			A		
Innovative Materials & Technologies for Sustainable Water Purification *(ENVR)			D	DE	D
Green Chemistry Adoption: Progressive Changes by Different Industry Sectors *(ENVR)			D		
GSSPC: Water Sustainability *(CHED)			D		
Science & Perception of Climate Change *(ENVR)			P	E	
Advances in Resource Recovery & Conservation in Water Systems *(ENVR)				PE	D

Committee on Ethics — ETHX

K. Vitense, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit *(CINF)		P			

International Activities Committee — IAC

E. Contis, Program Chair

Hotel Nikko San Francisco	S	M	Tu	W	Th
Blending Chemistry & Culture: Undergraduate Research Abroad Through ACS IREU Program **	D				
Teaching, Researching & Community Building in the Global Chemical Enterprise **		D			
Chemistry of Korean Foods & Beverages *(AGFD)	D				
International & Multicultural Perspective *(CHED)		P			
Perspectives on Climate Change Literacy & Education: Local to International *(CHED)			A		
Research on Learning in the Lab *(CHED)				A	

Committee on Local Section Activities — LSAC

M. Rudd, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Hollyweird Chemistry *(CPRC)	P	D			
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)		D			

Committee on Minority Affairs — CMA

J. Sarquis, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross *(WCC)	P		A		
ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in Honor of Saundra Y. McGuire *(CHED)			A		
Advancing Undergraduate Research *(CHED)			D	A	

Committee on Patents & Related Matters — CPRM

S. Shah, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit *(CINF)		P			

Committee on Public Relations and Communications — CPRC

D. Nelson, Program Chair

Moscone Center	S	M	Tu	W	Th
Hollyweird Chemistry **	P	D			
Space Chemistry: How It Helps Space Exploration *(YCC)		D			
Chemists & Writing for Fun & Profit: Write Your Own Career *(SCHB)			A		
Communicating Science in the 21st Century to Diversified Audiences *(CHED)				D	

Committee on Science — COMSCI

M. Kociolek, Program Chair

Moscone Center	S	M	Tu	W	Th
Chemical Innovation Partnerships: Industry-University Success Stories		P			

Senior Chemists Committee — SCC

T. Beattie, Program Chair

Located with Primary Sponsor	S	M	Tu	W	Th
Golden Age of Industrial Chemistry *(HIST)	P				

Society Committee on Education — SOCED

M. Roslonowski, Program Chair

San Francisco Marriott Marquis	S	M	Tu	W	Th
Frontiers in Nanoscience **	A				
Chemistry of Fermented Beverages		A			
Eminent Scientist Lecture with Dr. Carolyn Bertozzi **		P			
Undergraduate Research Papers *(CHED)	D	D			
Hollyweird Chemistry *(CPRC)	P	D			
Excellence in Graduate Polymer Research *(POLY)		D	DE		
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)		D			
Undergraduate Research Posters *(CHED)		P			
Successful Student Chapters *(CHED)		E			

Women Chemists Committee W C C

K. Woznack, R. Cole, Program Chairs

Hotel Nikko San Francisco	S	M	Tu	W	Th
The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross **	P		A		
Celebrating 90 years of the WCC: Reflections of Past Chairs **		A			
Rising Star Award Symposium **		P			
Lanthanide & Actinide Chemistry *(INOR)	A		E	A	D
ACS Award in Surface Chemistry: Symposium in Honor of Cynthia M. Friend *(CATL)	D	D			
ACS Award in Applied Polymer Science: Symposium in Honor of Zhenan Bao *(PMSE)	D	D			
High School Program *(CHED)	D				
F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in Honor of Pingyun Feng *(INOR)	DE	P			
ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Symposium in Honor of Marcy H. Towns *(CHED)		D			
ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in Honor of Saundra Y. McGuire *(CHED)			A		
Advancing Undergraduate Research *(CHED)			D	A	
Biomass & Biofuel Processing *(ENFL)			D	D	
ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in Honor of Yvonne C. Martin *(COMP)			D		
ACS Award Lectures *(COLL)			P		
ACS Chemical Biology Award Symposium *(BIOL)			P		
Frank H. Field & Joe L. Franklin Award for Outstanding Achievement: Symposium in Honor of Vicki H. Wysocki *(ANYL)			P		
Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in Honor of Junqi Li & Martin D. Burke *(ORGN)				A	
Chemical Probes for Bacterial Imaging *(BIOL)				P	

Younger Chemists Committee Y C C

D. Williams, Program Chair

Moscone Center	S	M	Tu	W	Th
Starting a Successful Research Program at a PUI **	P				
Entrepreneurial Opportunities in Chemistry **	E				
Space Chemistry: How It Helps Space Exploration ** AMTSP		D			
Hollyweird Chemistry *(CPRC)	P	D			
Golden Age of Industrial Chemistry *(HIST)	P				
Excellence in Graduate Polymer Research *(POLY)		D	DE		
Fundamentals of Chemistry Outreach Education: From Program Design to Assessment *(CHED)		D			
Looking Beyond Your Current Boundaries: What's the Next Step? *(PROF)				D	
Young Investigators in Nuclear & Radiochemistry *(NUCL)					D

*Cosponsored symposium with primary organizer shown in parentheses; located with primary organizer.
**Primary organizer of a cosponsored symposium.

AMTSP: Advanced Materials, Technologies, Systems & Processes
A = AM AE = AM/EVE P = PM D = AM/PM
E = EVE DE = AM/PM/EVE PE = PM/EVE

How to Read the Technical Program

1. Search for the Division— listed in alphabetical order

3. Locate the session name

4. Locate the time or poster #

GEOC

Division of Geochemistry

A. Ilgen, *Program Chair*

SUNDAY MORNING

Section A

San Francisco Marriott Union Square
Union Square North

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Cosponsored by COLL and ENVR

C. S. Kim, P. A. O'Day, *Organizers*

B. Gilbert, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 GEOC **1.** X-ray absorption spectroscopy studies of sorption reactions at mineral-aqueous

2. Locate the day

5. Locate the venue and room for each session

Note:
Times represent the start of oral presentations and numbers represent poster numbers.

‡ *Cooperative Cosponsorship*

FULL TECHNICAL PROGRAM

TWENTY-NINE OF THE SOCIETY'S technical divisions and six committees are hosting original technical programming during the meeting. More than 14,000 papers have been accepted for this meeting.

Each organizing group's programming is detailed on the following pages. Nearly 4,000 chemical professionals and students are expected to attend the ever-popular Sci-Mix Interdivisional Poster Session & Mixer on Monday, April 3 from 8:00 to 10:00 PM at Moscone Center, Hall D. More than 1,000 noteworthy poster presentations, networking with colleagues, and light refreshments make up this enjoyable event.

PRES

Presidential Events

A. Campbell, *Program Chair*

SUNDAY MORNING

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

PHYS Division Awards Symposium

Ahmed Zewail Award in Ultrafast Science & Technology: Symposium in honor of Stephen R. Leone

Sponsored by PHYS, Cosponsored by PRES

SUNDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Salon 8

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

A. Campbell, *Organizer*

C. J. Burrows, *Organizer, Presiding*

1:20 Introductory Remarks.

1:30 PRES **1.** New opportunities for using light in energy conversion. **A. Alivisatos**

2:00 PRES **2.** Challenges and opportunities for synthetic chemists in grid-scale energy storage. **M.S. Sanford**

2:30 PRES **3.** Electrochemical and chemical storage of electrons at nanoscale for sustainable future. **Y. Cui**

3:00 PRES **4.** Defining the glycome, the final omics frontier. **C.R. Bertozzi**

3:30 PRES **5.** Controlling silica in its crystalline and amorphous states: A problem in surface science. **H. Freund**

Best Practices in Selecting & Presenting Safety Training Content

Sponsored by CHAS, Cosponsored by CCS and PRES

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodolgies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

PHYS Division Awards Symposium

Ahmed Zewail Award in Ultrafast Science & Technology: Symposium in Honor of Stephen R. Leone

Sponsored by PHYS, Cosponsored by PRES

MONDAY MORNING

Section A

Moscone Center

133

Science for a Sustainable Energy Future

Energy Storage

Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Financially supported by Chemical Sciences Roundtable; SSURF

A. Campbell, *Organizer, Presiding*

8:30 Introductory Remarks: A. Campbell.

8:40 Discussion: Energy Research: S. Binkley.

9:05 PRES **7.** Challenges for large scale energy storage and transmission. **J. Liu**

9:35 PRES **8.** How flexible long-duration storage is changing the way energy storage is used. **J. Song**

10:05 PRES **9.** Developing and applying new tools to understand how materials for Li and beyond-Li battery technologies function. **C.P. Grey**

10:35 PRES **10.** Innovation in stationary electricity storage: The liquid metal battery. **D.R. Sadoway**

11:05 PRES **11.** Storing energy in lithium batteries for a sustainable energy future. **M. Whittingham**

11:35 Panel Discussion.

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

Celebrating 90 years of the WCC: Reflections of Past Chairs

Sponsored by WCC, Cosponsored by PRES and PROF

Chemical Forensics

Investigations of Alleged Use & Source Attribution of Chemical Weapons

Sponsored by ANYL, Cosponsored by CHAL and PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

PHYS Division Awards Symposium

Peter Debye Award in Physical Chemistry: Symposium in honor of Bruce J. Berne

Sponsored by PHYS, Cosponsored by PRES

MONDAY AFTERNOON

Section A

Moscone Center

133

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

A. Campbell, *Organizer, Presiding*

1:30 Introductory Remarks.

1:40 PRES **12.** Exploiting anaerobes for biomass breakdown and sustainable chemistry. **M.A. O'Malley**

2:10 PRES **13.** Driving the future: The development of advanced biomass conversion technologies at the Joint BioEnergy Institute. **B.A. Simmons**

2:40 PRES **14.** Designer interfaces for energy storage and recovery. **Y. Surendranath**

3:10 PRES **15.** Novel strategies to enhance catalytic vectors. **J.A. Lercher**

3:40 PRES **16.** Role of innovation in enabling a sustainable energy future. **D.E. Arvizu**

4:10 Panel Discussion.

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Chemical Forensics

Chemical Attribution Signatures of Illicit Drugs & Toxic Chemicals

Sponsored by ANYL, Cosponsored by CHAL and PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

PHYS Division Awards Symposium

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids: Symposium in honor of Salvatore Torquato

Sponsored by PHYS, Cosponsored by PRES

Rising Star Award Symposium

Sponsored by WCC, Cosponsored by BIOL and PRES

TUESDAY MORNING

Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators

Sponsored by PROF, Cosponsored by BMGT, CHED and PRES

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Sponsored by NUCL, Cosponsored by INOR and PRES

Chemical Forensics

Chemometrics & Statistics for Signature Discovery & Exploitation

Sponsored by ANYL, Cosponsored by CHAL and PRES

GSSPC: Water Sustainability

Chemists in Pursuit of Clean Water

Sponsored by CHED, Cosponsored by CEI and PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

PHYS Division Awards Symposium

ACS Award in Theoretical Chemistry: Symposium in honor of Peter Pulay

Sponsored by PHYS, Cosponsored by PRES

TUESDAY AFTERNOON

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Sponsored by NUCL, Cosponsored by INOR and PRES

Chemical Forensics

Isotopic & Elemental Profiling for the Source Attribution of Materials

Sponsored by ANYL, Cosponsored by CHAL and PRES

GSSPC: Water Sustainability

Chemists in Pursuit of Clean Water

Sponsored by CHED, Cosponsored by CEI and PRES

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

PHYS Division Awards Symposium

E. Bright Wilson Award: Symposium in honor of David J. Nesbitt

Sponsored by PHYS, Cosponsored by PRES

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Chemists Leading the Charge: Chemists Using Business Acumen & Transformative Research to Address Societal Needs

Sponsored by INOR, Cosponsored by BMGT‡, MPPG, PRES and PROF‡

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

TUESDAY EVENING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY MORNING

What Have We Learned & Where Are We Going: Post-Settlement in the University of California

Sponsored by CHAS, Cosponsored by CCS and PRES

Communicating Science in the Twenty-First Century to Diversified Audiences

Sponsored by CHED, Cosponsored by CPRC, CWD and PRES

PHYS Division Awards Symposium

Francis P. Garvan–John M. Olin Medal: Symposium in honor of Barbara J. Finlayson-Pitt

Sponsored by PHYS, Cosponsored by PRES

WEDNESDAY AFTERNOON

What Have We Learned & Where Are We Going: Post-Settlement in the University of California

Sponsored by CHAS, Cosponsored by CCS and PRES

Communicating Science in the Twenty-First Century to Diversified Audiences

Sponsored by CHED, Cosponsored by CPRC, CWD and PRES

THURSDAY MORNING

Current Best Practices for Chemistry REU Programs

Sponsored by CHED, Cosponsored by PRES

MPPG

Multidisciplinary Program Planning Group

K. Beers, *Program Chair*

SUNDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 302

Spotlight on Advanced Materials, Technologies, Systems & Processes in the Journal of the American Chemical Society

S. Krane, *Organizer, Presiding*

P. J. Stang, *Presiding*

8:30 Introductory Remarks.

8:35 MPPG **1.** Advanced bioelectrocatalytic materials for fuel cells and electrosynthesis. **S.D. Minteer**

9:10 MPPG **2.** Surface coordination chemistry of metal nanomaterials. **N. Zheng**

9:45 MPPG **3.** From upconverting nanoparticles to graphene: When surfaces matter. **M. Cerruti**

10:20 MPPG **4.** Semiconductor nanowires for energy conversion. **P. Yang**

10:55 MPPG **5.** Fluorescent nanodiamonds for precision sensing & drug delivery applications. **T. Weil**

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Polymeric Materials for Performance & Sustainability

Biobased Polymers

Sponsored by POLY, Cosponsored by MPPG‡

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Catalysis for Unconventional Energy Sources

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Incorporating Polymer Science into the Classroom

Undergraduate Curriculum

Sponsored by POLY, Cosponsored by CHED, MPPG‡ and PMSE

Computations for CO_2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

SUNDAY AFTERNOON

Section B

Moscone Center

Gateway Ballroom 103/104

Advanced Materials, Technologies, Systems & Processes Plenary Session

K. Beers, *Organizer, Presiding*

3:00 MPPG **6.** Clean energy challenge: An integrated approach involving basic research, innovation and human factors. **P.F. Green**

3:45 MPPG **7.** Technology at the interface of microelectronics, life sciences, and big data: Materials challenges. **J.G. Linhardt**

4:30 MPPG **8.** From design and synthesis to advanced properties and sustainable polymeric materials. **A. Albertsson**

5:15 MPPG **9.** Fostering industrial and academic partnerships. **K. Watson**

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Polymeric Materials for Performance & Sustainability

Functional Materials: Gels & Membranes

Sponsored by POLY, Cosponsored by MPPG‡

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Catalysis for Unconventional Energy Sources

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Incorporating Polymer Science into the Classroom

High School & Community College

Sponsored by POLY, Cosponsored by CHED, MPPG‡ and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage

Cathode Materials

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Computations for CO_2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY MORNING

Section A

Moscone Center

130

Advanced Materials, Technologies, Systems & Processes: Implementation of Chemistry into Practice

K. Beers, *Organizer, Presiding*

8:45 Introductory Remarks.

8:55 MPPG **10.** Designing organic semiconductors for advanced applications. **M. Jeffries-El**

9:25 MPPG **11.** Opportunities for new and efficient catalytic processes for the utilization of natural gas. **T. Gunnoe**, M.S. Webster-Gardiner, B.A. Vaughan, S.K. Khani, J.B. Gary, J. Chen, B.A. McKeown, T.R. Cundari

9:55 MPPG **12.** Automated flow peptide synthesis: Toward amide bonds at nature's pace. **B.L. Pentelute**

10:25 MPPG **13.** Chemistry in a startup envionment: A personal journey. **C. Reich**

10:55 MPPG **14.** Making real parts: Rethinking materials for 3D manufacturing. **J. Rolland**

11:25 MPPG **15.** Modifying organic polymers using metal-organic materials: A perspective from a Fulbright fellow in Peru. **C.V. Gauthier**, S. Kim, J. Nakamatsu

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Polymeric Materials for Performance & Sustainability

High Performance

Sponsored by POLY, Cosponsored by MPPG‡

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Catalysis for Unconventional Energy Sources

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Innovative Chemistry & Materials for Electrochemical Energy Storage

Flow Batteries & Organic Electrodes

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

50th Anniversary Celebration of Macromolecules

Sponsored by POLY, Cosponsored by MPPG‡ and PMSE

Computations for CO_2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY AFTERNOON

Section A

Moscone Center

130

Nanoscience & Nanotechnology for Advanced Materials & Technologies

L. E. Fernandez, *Organizer*

P. Alivisatos, P. S. Weiss, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:10 MPPG **16.** Nanoscale gems, needles and grooves. **H. Park**

1:45 MPPG **17.** Exploiting the nanocrystal library to construct electronic and optoelectronic devices. **C.R. Kagan**

2:20 MPPG **18.** Carbon dots for environmental and energy applications. Z. Kang, **S. Lee**

2:55 MPPG **19.** Structure-controlled synthesis of single-walled carbon nanotubes. **Y. Li**

Section B

Moscone Center

Gateway Ballroom 103/104

The Kavli Foundation Emerging Leader in Chemistry Lecture

A. Campbell, *Organizer, Presiding*

4:00 Introductory Remarks.

4:05 MPPG **20.** Classical challenges in the physical chemistry of polymer networks. **B.D. Olsen**, J.A. Johnson, R. Wang, S. Tang, M. Zhong, K. Kawamoto, J. Ramirez, T. Dursch

4:55 Q&A Session.

Section B

Moscone Center

Gateway Ballroom 103/104

The Fred Kavli Innovations in Chemistry Lecture

A. Campbell, *Organizer, Presiding*

5:15 Introductory Remarks.

5:20 MPPG **21.** CRISPR systems: Nature's toolkit for genome engineering. **J. Doudna**

6:15 Q&A Session.

Industrial Innovations in Polymer Chemistry

Sponsored by POLY, Cosponsored by MPPG‡ and PMSE

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Polymeric Materials for Performance & Sustainability

Biodegradable & Recyclable Polymers

Sponsored by POLY, Cosponsored by MPPG‡

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Innovative Chemistry & Materials for Electrochemical Energy Storage

Capacitors

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

50th Anniversary Celebration of Macromolecules

Sponsored by POLY, Cosponsored by MPPG‡ and PMSE

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

TUESDAY MORNING

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Polymers under Deformation

Structure & Morphology Changes during Deformation of Polyolefins & Polymer Composites

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Polymeric Materials for Performance & Sustainability

Functional Materials for Energy & Electronics

Sponsored by POLY, Cosponsored by MPPG‡

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage

Solid-State Electrolytes & Beyond Li

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

Polymer Chemistry (RSC) Lectureship

Sponsored by POLY, Cosponsored by MPPG‡

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Materials Chemistry of Solutions & Solids for a Sustainable Future

Sponsored by INOR, Cosponsored by BMGT‡, MPPG, PRES and PROF‡

Chemistry is Central to Applied Materials

Sponsored by INOR, Cosponsored by MPPG‡

TUESDAY AFTERNOON

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Polymers under Deformation

Applying Advances in Characterization Methods for In-Situ Studies of Deformation

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Advances in Polysaccharides: Practice & Applications

New Developments in the Industrial Sector

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Innovative Chemistry & Materials for Electrochemical Energy Storage

2D Energy Storage Materials

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

Polymer Chemistry (RSC) Lectureship

Sponsored by POLY, Cosponsored by MPPG‡

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Chemists Leading the Charge: Chemists Using Business Acumen & Transformative Research to Address Societal Needs

Sponsored by INOR, Cosponsored by BMGT‡, MPPG, PRES and PROF‡

WEDNESDAY MORNING

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Polymers under Deformation

AFM & Nanoindentation Studies

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Advances in Polysaccharides: Practice & Applications

Novel Biocatalytic & Biopolymeric Approaches

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Polymeric Materials for Performance & Sustainability

Other Functional Materials

Sponsored by POLY, Cosponsored by MPPG‡

Innovative Chemistry & Materials for Electrochemical Energy Storage

Electrolytes & Interface

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

Undergraduate Laboratory Experiments Involving Advanced Materials

Sponsored by CHED, Cosponsored by MPPG‡

Chemistry is Central to Applied Materials

Sponsored by INOR, Cosponsored by MPPG‡

WEDNESDAY AFTERNOON

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

‡ *Cooperative Cosponsorship*

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Polymers under Deformation

Control of Deformation across the Length Scale for Advanced Polymer Materials

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Advanced Materials & Structures

Sponsored by CELL, Cosponsored by MPPG‡ and POLY

Advances in Polysaccharides: Practice & Applications

Novel Materials & Methodologies

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Polymeric Materials for Performance & Sustainability

Recylable & Bio-Based Materials

Sponsored by POLY, Cosponsored by MPPG‡

Innovative Chemistry & Materials for Electrochemical Energy Storage

Anode Materials & Li-S

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

Undergraduate Laboratory Experiments Involving Advanced Materials

Sponsored by CHED, Cosponsored by MPPG‡

Frontiers in Glycoanalytics

MS & NMR Methods

Sponsored by CELL, Cosponsored by ANYL, CARB‡ and MPPG‡

THURSDAY MORNING

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Next Generation Smart Materials

Sponsored by POLY, Cosponsored by MPPG‡

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Commercial & Versatile Technology

Sponsored by CELL, Cosponsored by MPPG‡ and POLY

Advances in Polysaccharides: Practice & Applications

New Functional Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Polymeric Materials for Performance & Sustainability

Applications

Sponsored by POLY, Cosponsored by MPPG‡

Innovative Chemistry & Materials for Electrochemical Energy Storage

Electrochemical Catalysis & Energy Conversion

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Frontiers in Glycoanalytics

Molar Mass & Crystallinity Analyses

Sponsored by CELL, Cosponsored by ANYL, CARB‡ and MPPG‡

THURSDAY AFTERNOON

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Energy, Food & Packaging Development

Sponsored by CELL, Cosponsored by MPPG‡ and POLY

Advances in Polysaccharides: Practice & Applications

Preparation, Characterization & Applications

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

AGFD

Division of Agricultural and Food Chemistry

N. Seeram, *Program Chair*

SOCIAL EVENTS:

Poster Reception, 5:00 PM: Sun

BUSINESS MEETINGS:

Business Meeting, 12:00 PM: Tue

Future Program Meeting, 12:00 PM: Mon

SUNDAY MORNING

Section A

Hilton San Francisco Union Square

Continental Parlor 9

Chemistry & Biological Effects of Maple Food Products

H. Ma, N. P. Seeram, *Organizers*, *Presiding*

9:00 Introductory Remarks.

9:05 AGFD **1.** Maple-Derived food bioactives in human health & diseases: The path forward. **N.P. Seeram**

9:35 AGFD **2.** Effect of the new high vacuum technology on the chemical composition of maple sap and syrup. **L. Lagace**, M. Deschênes, N. Martin, F. Ethier, M. Beaudoin, J. Houde, S. Corriveau, M. Sadiki

10:05 AGFD **3.** Maple sugar, an unexplored maple food product: UFLC-TOF-MS/MS Characterization and neuroprotective activities of phenolics. **Y. Liu**, K. Rose, N.P. Seeram

10:35 Intermission.

10:50 AGFD **4.** Phenolic-enriched Maple Syrup Extract (MSX) inhibited the formation of advanced glycation end-products through its antioxidation capacity. **W. Liu**, H. Ma, Z. Wei, J. Dain, N.P. Seeram

11:20 AGFD **5.** Synthesis and characterization of the bioactivity of quebecol and its analogs. **N. Voyer**, S. Cardinal, C. Bouchard, D. Grenier

11:50 AGFD **6.** Unraveling the complex carbohydrates in maple syrup. **D.C. Rowley**, J. Sun, H. Ma, N.P. Seeram

12:20 Concluding Remarks.

Section B

Hilton San Francisco Union Square

Franciscan A

Chemistry of Korean Foods & Beverages

Cosponsored by IAC

C. H. Do, A. M. Rimando, *Organizers*

K. G. Lee, *Organizer, Presiding*

Y. Kim, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **7.** Introduction of Korean foods and beverages. **C.H. Do**, J.C. Park, S. Chun

8:30 AGFD **8.** Evaluation of metabolites from lactic acid bacteria originated from kimchi. **J. Lee**

8:55 AGFD **9.** Withdrawn.

9:20 AGFD **10.** Isolation and characterization of lactic acid bacteria from naturally fermented Korean sourdough. **N. Han**, C. Park, S. Shim, J. Seo

9:45 Intermission.

10:00 AGFD **11.** Lactic acid bacteria isolated from kimchi as a modulator of gut microbiota in diet-induced obese mice. **H. Choi**

10:25 AGFD **12.** Structure and function of garlic derived organo-sulfur compounds. **T. Seki**, T. Hosono

10:50 AGFD **13.** Reduction of food hazards in Maillard reaction based Korean food model systems. **K.G. Lee**

Section C

Hilton San Francisco Union Square

Franciscan B

Undergraduate Symposium

Cosponsored by CHED

K. D. Deibler, *Organizer*

A. E. Mitchell, *Presiding*

9:00 Introductory Remarks.

9:05 AGFD **14.** Detection of *Escherichia coli in drinking water using engineered bacteriophage*. **A. Chen**

9:30 AGFD **15.** Detection of 2,4-dichlorophenoxyacetic acid in food using molecularly imprinted polymers–surface enhanced Raman spectroscopy. **Z.M. Hua**

9:55 Intermission.

10:10 AGFD **16.** BG-4, a novel bioactive peptide from *Momordica charantia*, inhibits lipopolysaccharide-induced inflammation in THP-1 human macrophages. **L. Jones**, P. Pangloli, H. Krishnan, V.P. Dia

10:35 AGFD **17.** Investigation of antioxidant capacity and bioactive chemicals in South Carolina grown peaches. **R.F. Ramey**, F. Chen, L. Wang, C. Zhang, A. McCullogh, A. Burgess, T. Nguyen

11:00 AGFD **18.** Isolation and structure elucidation of bioactive compounds from *Garcinia buchananii seeds*. **B. Stiglbauer**, T.D. Stark

Nanocellulose Processing & Analysis

Novel Processes

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by AGFD

SUNDAY AFTERNOON

Section A

Hilton San Francisco Union Square

Continental Parlor 9

Chemistry & Biological Effects of Maple Food Products

H. Ma, N. P. Seeram, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **19.** Further investigations into the neuroprotective effects of a phenolic-enriched Maple Syrup Extract (MSX). **H. Ma**, N. DaSilva, S. Johnson, W. Liu, J. Dain, N.P. Seeram

1:35 AGFD **20.** Maple syrup reduces neurodegeneration in *C. elegans* models of amyotrophic lateral sclerosis. C. Bretonneau, C. Aaron, G. Beaudry, M. Therrien, A.**J. Parker**

2:05 AGFD **21.** Phenolic rich maple syrup extracts synergize with antibiotics. **N. Tufenkji**, V. Maisuria

2:35 Intermission.

2:50 AGFD **22.** Symbiotic maple saps minimize disruption of the mice intestinal microbiota after oral antibiotic administration. R. Hammami, N.B. Abdallah, J. Barbeau, **I. Fliss**

3:20 AGFD **23.** Food grade phenolic-enriched maple syrup extract (MSX) exerts protective effects against diet-induced hepatic-steatosis in mice. **A. Slitt**, H. Ma, N. DaSilva, C. Picard, M. Pfohl, E. Martell, M. Abustan, N.P. Seeram

3:50 AGFD **24.** Substituting sucrose for an equivalent amount of maple syrup and other natural sweeteners reduces metabolic syndrome and liver steatosis in a rat model of diet-induced obesity. M. Valle, P. St-Pierre, G. Pilon, F.F. Anhê, T. Varin, **A. Marette**

4:20 Concluding Remarks.

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Section B

Hilton San Francisco Union Square
Franciscan A

Chemistry of Korean Foods & Beverages

Cosponsored by IAC

A. M. Rimando, *Organizer*

C. H. Do, K. G. Lee, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **25.** Changes in phytochemicals, aroma compounds, and sensory properties of Korean teas influenced by harvesting time and oxidative fermentation. **Y. Kim**

1:30 AGFD **26.** Elucidation of flavor characteristics of Korean traditional fermented sauces. **Y. Kim**, S. Lee, M. Park, H. Namgung, K. Lee, S. Kum, S. Kim, J. Lee

1:55 AGFD **27.** Correlation between the physiochemical components and sensory properties of *Makgeolli*. **J. Kang**, H. Choi, C. Kim, S. Yeo, S. Jeong

2:20 AGFD **28.** Changes of volatile compositions in *soju* mashes from fermentation to distillation using different kinds of fermentation starters. **S. Lee**, K. Shin

2:45 Intermission.

3:00 AGFD **29.** Comparing the effects of high hydrostatic pressure and thermal pasteurization on the quality of soft-persimmon juice. **G. Kim**, J. Kim, K. Kim, S. Choi

3:25 AGFD **30.** Keeping kimchi delicious and safe through kimchi packaging. **S. Yoo**

3:50 AGFD **31.** Image-based high content screening assay to predict of hepatotoxicity of bioactive compounds in natural products. **H. Chun**

4:15 Discussion.

Section C

Hilton San Francisco Union Square
Franciscan B

Withycombe-Charalambous Graduate Student Symposium

Cosponsored by CHED

K. D. Deibler, *Organizer*

B. Park, *Presiding*

1:00 Introductory Remarks.

1:10 AGFD **32.** Novel polysaccharide-polypeptides nanocomplexes: Assembly, characterization, and encapsulation of polyphenol in multi-platforms. **Y. Jiang**, Q. Huang

1:40 AGFD **33.** Influence of legume proteins on the gastrointestinal digestion of omega-3 emulsions. **C. Gumus**, D. McClements

2:10 Intermission.

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

2:20 AGFD **34.** Prevention of obesity and type 2 diabetes with aged citrus peel (*chenpi*) extract. **J. Guo**, H. Tao, S. Jin, C. Ho, Q. Huang

2:50 AGFD **35.** Rapid detection of methicillin-resistant *Staphylococcus aureus* in pork using a nucleic acid-based lateral flow immunoassay. **L. Ma**, H. Zhang, L. Ma, Z.M. Hua, S. Wang, X. Lu

3:20 AGFD **36.** Absorption and metabolism of 3-MCPD 1-monopalmitate in rats. **B. Gao**, L.L. Yu

3:50 AGFD **37.** Synergistic inhibitory effect of allyl isothiocyanate and sulforaphane on human non-small cell lung carcinoma cells. **K. Rakariyatham**, Z. Gao, H. Xiao

Nanocellulose Processing & Analysis

Process Parameters

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by AGFD

SUNDAY EVENING

Section A

Moscone Center
West Hall

General Posters

N. P. Seeram, *Organizer*

5:00 - 7:00

AGFD **38.** Spatial variations in mercury and selenium concentrations in marine fishes of Rhode Island: Risks and benefits to human health. **J. Jacques**, M. Yurkevicius, D.L. Taylor

AGFD **39.** Rheology and microstructure of caseinate-based edible films. **M.H. Tunick**, L. Bonnaillie, L.D. Aburto, J. Mulherin, P.M. Tomasula

AGFD **40.** Fatty acid profiles of marine fishes from Rhode Island coastal waters. **M. Yurkevicius**, J. Jacques, N.E. Breen, D.L. Taylor

AGFD **41.** Cuticular hydrocarbon profile analysis of *Drosophila athabasca*: Variability by race. **B.L. Gay**, R. Yukilevich, J.D. Kehlbeck

AGFD **42.** Investigation of the kinetics and equilibrium chemistry of cold-brew coffee: Caffeine and chlorogenic acid concentrations as a function of roasting temperature and grind size. **N.Z. Rao**, M. Fuller, N. Parenti, S. Ryder, N. Setchie Tchato

AGFD **43.** Triterpenoid-enriched fruit extract of *Eugenia Jambolana L.* (Jamun) attenuates experimental type I diabetes in mice. Y. Zhao, R. Guo, Q. Zhang, Z. Guo, F. Xue, **J. Xu**

AGFD **44.** Effect of substitution of β-glucans on the glycemic response and thermal properties of common starches. **A. Anderson**

AGFD **45.** Vibrational spectroscopy and multivariate data analysis for elucidation and classification of compositional changes in milk subject to Supercritical Fluid Extraction (SFE). E. Jones, **C. Ulrichsen**, A. Laubscher, R. Jimenez-Flores

AGFD **46.** Mechanistic investigation of nitrification inhibition and subsequent nitrous oxide (N2O) emission. **S. Li**, G. Chen

AGFD **47.** Novel collagen-derived glycopeptide pro-Hyp-CONH-GlcN: Synthesis and transepithelial transport in Caco-2 cell model. **M. Feng**, M. Betti

AGFD **48.** Effect of drying in raw almonds with concealed damage. **C. Rogel-Castillo**, **A.E. Mitchell**

AGFD **49.** Determination of raffinose content in pulses as a factor enhances the growth of probiotics and antioxidant protection in yogurt. **P. Dinh**, K. Bhargava, S. Gamagedara

AGFD **50.** Detection of polyphenolic compounds in crude extract samples of strawberry cultivars. **C.M. Van Spronsen**, N.C. Dopke

AGFD **51.** Vapor-Infusion of wine flavor volatiles in specialty dark chocolate and analysis via GC-MS. **S. Richards**, P.J. Iles, L.D. Giddings, R.V. Valcarce, N.R. Bastian, R. Holcomb, R. Mcfarland, H. Hsieh, T. Nielsen, J. Reelitz, M. Alvarez, S. Cunnginham

AGFD **52.** Optical control of insecticide activity and insect behaviors. **S. Xusheng**, Z. Gao, Y. Feng

AGFD **53.** Reduction of lead uptake in leafy green vegetables using an ion exchange material. **A. Anthony**, **M. Schenkel**, L. Taormina, C.C. Philipp

AGFD **54.** Comparison of fruit quality and metabolite profiling of natural or exogenous ethylene-induced ripe kiwifruit Jecy green. S. Lim, J. Lee, **E. Lee**

AGFD **55.** Comparison of amygdalin levels in California almond (*Prunus dulcis*) varietals using UHPLC-(ESI) QqQ MS/MS. **K. Luo**, A.E. Mitchell

AGFD **56.** Sugar and organic acid content of astringent, non-astringent, and pollination variant persimmons. **A.M. Vilches**, I.J. Sedej, C.W. Olsen, J. Smith, R.D. Woods, J.E. Preece, R.R. Milczarek, **A.P. Breksa**

AGFD **57.** Vapor-Infusion of whiskey flavor volatiles in specialty dark chocolate and analysis via GC-MS. **S. Richards**, P.J. Iles, L.D. Giddings, R. Holcomb, N.R. Bastian, R.V. Valcarce, M. Alvarez, R. Mcfarland, H. Hsieh, J. Reelitz, T. Nielsen, S. Cunnginham

AGFD **58.** Dynamics and imbalance of nutrient concentrations in a closed hydroponic system during tomato growth. J. Lee, A. Rahman, H. Azam, H. Kim, **M. Kwon**

AGFD **59.** Synthesis of cooper, iron, calcium and barium alginate beads for the controlled release of a systemic fungicide. **R. Torres Caban**, J. Munoz, F. Roman, L. Morell

AGFD **60.** Combinatorial enzyme technology for the conversion of agricultural fibers to functional products. **S.B. Batt Throne**, D. Feng, W.J. Orts, D.W. Wong

AGFD **61.** Combinatorial enzyme technology: Conversion of pectin to oligo species and its effect on microbial growth. **D. Feng**, S.B. Batt Throne, W.J. Orts, D.W. Wong

AGFD **62.** Dissipation pattern of pesticide residues during cultivation of agricultural products for establishing post-harvest residue level in Korea. **J. Park**, S. Yang, H. Choi

AGFD **63.** Aroma optimization of low caloric, alcohol-free beverages. **D. Gernat**, E. Brouwer, M. Ottens

AGFD **64.** Estimation of capsaicin and other nutritionally important compounds in Colorado grown pepper cultivars. **M. Hamed**, D. Kalita, M. Bartolo, S. Jayant

AGFD **65.** Biochemical characterization of the polyphenolic radical in third hand smoke. A. Skochko, C. Lopez, S. Russell, G. Firestone, **K. Stone**

AGFD **66.** Changes of volatile flavors during fermentation of kimchi. **W. Hawer**, D. Seo

AGFD **67.** Environmental extraction and quantitation of tetracycline antibiotics and their metabolites in agricultural wates using SPE, HPLC-MS, and HPLC-PDA. **A.J. Abdulrheem**, C. Fullington, J.H. Loughrin, E.D. Conte

AGFD **68.** Macro and micro-mineral contents of the pork cuts in Korea. **D. Seo**, S. Kim, J. Hwang, H. Lee, J. Park, Y. Jin, Y. Choi, S. Kim, J. Nam

AGFD **69.** Experiment for analysis of urushiol in sumac and several indigenous food in Korea. **D. Seo**, K. Kim, W. Hawer

AGFD **70.** Mineral nutrient contents of lentil bean, khorasan wheat and quinoa. **J. Hwang**, D. Seo, S. Kim, H. Lee, J. Park, Y. Jin, Y. Choi, S. Kim, J. Nam

AGFD **71.** Effect of black rice on quality characteristics and antioxidant activity of yogurt fermented using *Lactobacillus paracasei* and *Lactobacillus rhamnosus*. **J. Yoon**, H. Kim, D. Baek, K. Choi, S. Ahn, C. Ra, J. Jhoo, G. Kim

AGFD **72.** Anti-allergic effects of low-molecular-weight peptides derived from bovine β-casein on RBL-2H3 cells. **H. Kim**, S. Park, S. Ahn, H. An, S. Yoon, G. Kim, J. Jhoo

AGFD **73.** Novel approaches to the chemical preparation and spectral characterization of tormentic acid. **Y. Lo**, G. Ren, J. Wu, **H. Honda**, T. Wei

AGFD **74.** Novel approaches to the chemical synthesis and biological activity of 24-ketolanosterol as an inhibitor of HMG-CoA reductase. E.J. Parish, **G. Ren**, Y. Lo, **H. Honda**

AGFD **75.** Novel approaches to the chemical synthesis and carbon-13 nuclear magnetic resonance spectral properties of cholest-4-en-3,6-dione. **D. Ren**, E.J. Parish, G. Ren, Y. Lo, **H. Honda**

AGFD **76.** Novel approaches to the chemical synthesis and structural characterization of hydroxysterols. E.J. Parish, Y. Lo, **H. Shyu**, **H. Honda**, T. Wei

AGFD **77.** Multiplex surface plasmon resonance imaging platform for label-free detection of foodborne pathogens. **J. Chen**, B. Park

AGFD **78.** Effect of the cocoa butter equivalent addition on the volatile compounds of dark chocolate. C. Silva de Souza, **J. Block**

AGFD **79.** Characterization of chemical and biological properties of proanthocyanidins from color corn after different processing methods. **C. Chen**, P. Somavat, V. Singh, E.G. Demejia

AGFD **80.** Low-resolution 1H NMR as a reliable technique to study fresh and freeze-thawed hen egg yolk. C. Au, T. Wang, **N. Acevedo**

AGFD **81.** Elucidation of the gelation mechanism of frozen-thawed egg yolk. C. Au, **N. Acevedo**, T. Wang

AGFD **82.** Cellulose nanocrystals with light induced antimicrobial functions. **Y. Zhu**

AGFD **83.** Encapsulation of microbial isolates in alginate beads designed to increase nutrient uptake in hydroponic systems. **F. Al Jallaf**, H.H. Hernandez

‡ *Cooperative Cosponsorship*

AGFD **84.** Quality characteristics of yogurt supplemented with trehalose and fructooligosaccharide. **D. Baek**, H. An, J. Park, J. Jhoo, G. Kim

AGFD **85.** Phenolic profile of aqueous and hydroalcoholic extracts from pecan nut shell [*Carya illinoinensis* (Wangenh) C.Koch] obtained by optimization of ultrasonic-assisted extraction. **J. Block**, J. Hilbig, J. Bork

AGFD **86.** Sagebrush polyphenols impact the expression of CYP1A1. **S. Nosworthy**, J. Forbey, R. Prough, C. Dadabay

AGFD **87.** Isolation and purification of sesquiterpene lactones in sagebush. **C.E. Ferrell**, J. Forbey, C. Dadabay

AGFD **88.** Antioxidant properties and phenolic concentrations of herbs within the Lamiaceae family. **J. Ahn**, **A. Alford**, E.D. Niemeyer

AGFD **89.** Green synthesis of coumarin derivatives in search of potent pesticides for sustainable agriculture. **M. Uroos**, N. Akhtar, J. Tariq

AGFD **90.** Chemical composition, and antinutritional factors in seeds, cake, and botanical fractions of Sacha inchi (*Plukenetia volubilis L.*). **P. Glorio**, M. Baquerizo, G. Rodríguez.Paucar, J. Chavez, R. Lazaro, F. Saldaña

AGFD **91.** Effect of plant maturity on antioxidant properties and phenolic concentrations in green basil (*Ocimum basilicum L.*) cultivars. **C. Palmer**, **A. Reddy**, E.D. Niemeyer

AGFD **92.** LC/MS-MS method optimization for the detection and quantification of moxidectin in bovine serum. **G. Samenuk**, A.A. Pérez de León, R. Miller

AGFD **93.** Effect of mechanical stress on anthocyanin levels in blackberries. **A. Anthony**, **C. Schoborg**, M. Schenkel, A. Kinman, C.C. Philipp

AGFD **94.** Influence of organophosphorus pesticides on the stability of plasmonic nanoparticles in the presence of dissolved organic matter. **N.M. Dissanayake**, S.O. Obare

AGFD **95.** Detection of microbial volatile organic compounds released from *Macrophmina phaseolina* by headspace solid phase mirco-extraction and gas chromatography-mass spectrometry. **J. She**

AGFD **96.** Chemical analysis of a commercial product containing essential oils shown to control southern cattle fever tick infestations in bovines. **M. Montoya**, S.B. Bach, A.A. Pérez de León, R. Miller

AGFD **97.** Changes in monoterpene glycosylation patterns in *Vitis vinifera* during grape berry maturation. **J. Godshaw**, A.K. Hjelmeland, J. Zweigenbaum, S.E. Ebeler

AGFD **98.** Density functional theory study on triplet intermolecular hydrogen transfer between cycloxydim and chlorothalonil. **Q. Yuan**, I.R. Gould, N. Kidley

AGFD **99.** Correlating micro climate to alpha and beta acid concentrations in hops. **R. Schindler**, **A. Chui**, Z. Sharrett, M. Lares

AGFD **100.** Proteomic characterization of inhalable dust from the California San Joaquin Valley. N. Nole, C. Santiago, **S. Russell**

AGFD **101.** Development and validation of QuEChERS method for simultaneous analysis of trichothecenes in nuts by ultra performance liquid Chromatography coupled to tandem mass spectrometry. **M. Yoo**, S. Lee, S. Kim

AGFD **102.** Novel metabolites of food contaminant phthalates revealed by HRMS and their implications in quantitating urinary toxicant exposure markers. J. Hsu, J. Hsu, Y. Chen, S. Tsai, **P. Liao**

AGFD **103.** Withdrawn.

AGFD **104.** Monitoring of natural preservative levels in fisheries products. **S. Lee**, M. Yoo, S. Choi, D. Shin

AGFD **105.** Development and application of the AMBER molecular mechanics force field to investigate herbicide interaction in plants. **T. Khanna**, L. Barter, I.R. Gould

AGFD **106.** Biological evaluation of Yansun (*Thunia alba L.*) extract from Yungui plateau in China. **H. Ma**, N.P. Seeram

AGFD **107.** Characterization of commercially available honey in Puerto Rico. **J. Becerra Lopez**, **R. Flores-Morales**, **A. Muñoz**, C. Perez-Rodriguez, M. Figueroa-Cruz, R. Maiz, K. Blanco, J. Morales-Velez, C. Camacho, J. Gomez-Torres, A. Vega Negron, A.M. Gonzalez

AGFD **108.** Ethanol analysis via infrared spectroscopy. **A. Campanella**, M.D. Mosher

AGFD **109.** Effects of cooling rate on g-oryzanol and β-sitosterol oleogels. **I. Hazlett**, N. Acevedo

AGFD **110.** Characterization of a novel arabinoxylan-glucan crosslink in rice bran fiber. **B.J. Savary**, K. Takahashi, K. Teoh

AGFD **111.** Determination of the effect of meringue under different conditions. **M. Nguyen**, E. Stemp

AGFD **112.** Analysis of major elements in wines using an Agilent MP-AES. **C.K. Tanabe**, H. Hopfer, R. Boulton, S.E. Ebeler, J. Nelson

AGFD **113.** Fast analysis of arsenic species in Californian wines with LC-ICP-QQQ. **C.K. Tanabe**, S.E. Ebeler, J. Nelson

AGFD **114.** Refrigeration storage of native and improved native potatoes. **F. Cerron Mercado**, P. Glorio-Paulet, F. Rodriguez, J. Nuñez

AGFD **115.** Characterization of the organoleptic properties, vitamin C levels and anti-oxidant contents of Californian grown persimmons. **I.J. Sedej**, A.M. Vilches, C.W. Olsen, J. Smith, R.D. Woods, J.E. Preece, R.R. Milczarek, A.P. Breksa

AGFD **116.** Industrial hemp for fuels and chemicals: From weed to wonder. S. Tulaphol, T. Phung, M. Hossain, N. Sun, T. Prasomsri, S. Renneckar, **N. Sathitsuksanoh**

AGFD **117.** Determination of imidacloprid in central California honey and the decline of the bee population. **S.C. Fleming**, B. Anderson, M. Barr-Ramsey, E. Issa, E. Manzo, D. Smith, M. Tjuanta, C. Olea

AGFD **118.** Palmitic, stearic and oleic acid sophorolipids and thiamine dilauryl sulfate inactivate *Escherichia coli* O157:H7 in the presence of low concentrations of ethanol. X. Zhang, R. Ashby, D. Solaiman, Y. Liu, **X. Fan**

AGFD **119.** Recovery of grape pomace polyphenols by polymeric adsorbents with affinity ligands and the evaluation of adsorption and desorption characteristics of polyphenols. **A. Seker**, S. Chen

AGFD **120.** Extraction and purification of (E)-resveratrol from the bark of conifer species in Maine. **P.S. Piyaratne**, B.W. Cole, R. Fort

MONDAY MORNING

Section A

Hilton San Francisco Union Square
Continental Parlor 9

Chemistry & Biological Activities of Phenolic Compounds from Fruits & Vegetables

Isolation, Food Composition & Antioxidant Activity

G. Gattuso, G. K. Jayaprakasha, *Organizers*

B. Patil, *Organizer, Presiding*

D. Barreca, V. Cheynier, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **121.** Concentration of polyphenolic compounds and antioxidant activity of garlic grown from air bulbils. A. Kopec, E. Jedrszczyk, R. Francik, **J. Zawistowski**

8:30 AGFD **122.** Changes of phenolic compounds resulting from thermal food processing. **S. Rohn**

8:55 AGFD **123.** Potential green solvents using accelerated extraction of Brussel sprouts yielded higher phenolics, antioxidant activity and -amylase inhibition. **G.K. Jayaprakasha**, H. S, Y.B. Ruiz, B. Patil

9:20 AGFD **124.** Cooking effects on the bioavailability and bioactivity of phenolic and carotenoids of Mediterranean sofrito. **R. Lamuela-Raventos**, J. Fernando-Rinaldi, S. Hurtado-Barroso, M. Martínez-Huélamo, M. Illan, X. Torrado

9:45 Intermission.

10:00 AGFD **125.** Natural and bioinspired phenol polymers with antioxidant properties for health and food applications. **A. Napolitano**

10:25 AGFD **126.** Analysis of non-extractable phenolic compounds in fruit products: Methodology and perspectives. **J. Pérez-Jiménez**, F. Saura-Calixto

10:50 AGFD **127.** Edible bean sprouts as a dietary source of antioxidant phenolics. **H. Corke**, R. Gan

11:15 Concluding Remarks.

Section B

Hilton San Francisco Union Square
Franciscan A

Artisanal Foods

A. L. Waterhouse, *Organizer*

M. H. Tunick, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 AGFD **128.** Marketing artisanal products. **R. Villarreal**

8:45 AGFD **129.** Impact on chemical composition of yerba mate tea using artisan methods in comparison to mass-produced technology. **E.G. Demejia**, D. Karr

9:30 Intermission.

9:45 AGFD **130.** Fundamentals of coffee brewing. **K. Sanchez**

10:05 AGFD **131.** Physics and chemistry of brewing coffee. **C. Hendon**

10:30 AGFD **132.** Craft and science of artisanal wine. **A.L. Waterhouse**, N. Gislason

Section C

Hilton San Francisco Union Square
Franciscan B

Structure & Chemistry of Proteins of Food Safety & Food Manufacturing Interest

Y. Zhang, *Organizer, Presiding*

8:00 AGFD **133.** Detection of allergens and gluten in fermented and hydrolyzed food and ingredients. **L. Jackson**

8:25 AGFD **134.** Nucleic acid-based sensors for the detection of gluten in food: A tool for ensuring the safety of celiac patients. **M. Lobo-Castañón**, R. Miranda-Castro, N. de-los-Santos-Alvarez, A.J. Miranda-Ordieres

8:50 AGFD **135.** Caracterización de sericina producido por liofilización. **C. Londoño**, **D.C. Castrillón Martínez**, **A. Restrepo**, **C. Alvarez**

9:15 AGFD **136.** Differences in the functionality and characterization of kafirins extracted from decorticated sorghum flour or gluten meal treated with protease. **J. Espinosa**, I. Garza-Guajardo, E. Perez-Carrillo, S.O. Serna-Saldivar

9:40 Intermission.

9:55 AGFD **137.** Recent development in typing, characterization and detection of Shiga toxins produced by pathogenic *E. coli*. **X. He**

10:20 AGFD **138.** Functionalization of food proteins and peptides via Transglutaminase (TGase) catalysis: Effects on bioactivity, functionality and safety. **M. Betti**, Y. Hrynets

10:45 AGFD **139.** Recent development in recombinant food allergen production. **Y. Zhang**

11:10 AGFD **140.** β-Lactoglobulin-chlorogenic acid conjugate-based nanoparticle for delivery of (–)-epigallocatechin-3-gallate. **J. Yi**, Y. Fan, Y. Zhang

Nanocellulose Processing & Analysis

Properties

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

MONDAY AFTERNOON

Section A

Hilton San Francisco Union Square
Continental Parlor 9

Chemistry & Biological Activities of Phenolic Compounds from Fruits & Vegetables

HPLC Separation, Mass Spectrometry & Antioxidant Activity

G. Gattuso, G. K. Jayaprakasha, B. Patil, *Organizers*

G. Gowda, R. Lamuela-Raventos, J. Singh, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **141.** Analytical characterization of anthocyanins in *Vaccinium myrtillus L.* berries and food products. **V. Brighenti**, C. Ranieri, F. Pellati, S. Benvenuti

1:30 AGFD **142.** Properties and applications of macromolecular antioxidants, the hidden face of dietary antioxidants. **F. Saura Calixto**, J. Pérez-Jiménez

1:55 AGFD **143.** High-resolution mass spectrometry analysis of flavonoid-acetaldehyde reaction products in wine-like model solutions. A. Vallverdu-Queralt, E. Meudec, R. Lamuela-Raventos, N. Sommerer, **V. Cheynier**

2:20 AGFD **144.** Polyphenolic profiles of fruits grown in Serbia. **Z. Tesic**, U. Gasic, D. Milojkovic-Opsenica

2:45 Intermission.

3:00 AGFD **145.** UHPLC-qTOF MS analysis of phenols in wines made with different maceration techniques. **S. Frost**, J. Blackman, J. Zweigenbaum, H. Heymann, S.E. Ebeler

3:25 AGFD **146.** Combination of green solvents using accelerated extraction of spinach and LC-HR-ESI-QTOF-MS led five new flavonoids and yielded higher antioxidants. J. Singh, **G.K. Jayaprakasha**, B. Patil

3:50 AGFD **147.** Determination of ellagic acid in the wastes of wallnut, chestnut and pomegranate grown in Turkey using HPLC-DAD method. **G. Yalcin**, C. Demirbag, I. Bahsi, L. Ozgul, D. Bilgic, H. Onurlu, S.A. Seyhan

4:15 Concluding Remarks.

Section B

Hilton San Francisco Union Square
Franciscan A

Artisanal Foods

M. H. Tunick, *Organizer*

A. L. Waterhouse, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **148.** Crafting a regionally evocative gin using locally wild-crafted botanicals. **D. Smith**, **T.S. Collins**

1:50 AGFD **149.** Mezcal: An ancestral distilled beverage obtained from agave. **A.C. Gschaedler**, M. Kirchmayr, M. Arellano, R. Prado

2:15 AGFD **150.** Artisanal excellence: Beer. **C. Bamforth**, S. Ungermann

3:00 Intermission.

3:15 AGFD **151.** Artisanal chocolate: Flavor chemistry of the enticing aroma and taste of cocoa. **M. Foley**

4:00 AGFD **152.** Volatile compounds during traditional fermentation and dying of cacao (Theobroma cacao). **E. Lugo**, A. Gschaedler, J. Rodriguez

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Section C

Hilton San Francisco Union Square
Franciscan B

General Papers

N. P. Seeram, *Organizer, Presiding*

H. Ma, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **153.** Withdrawn.

1:30 AGFD **154.** Bioassay-guided isolation and structure elucidation of a natural product inhibitor of *Xylella fastidiosa* from the endophytic fungus Ulocladium sp. **M. Papineau**, L. D'Elia, P. Rolshausen, C. Roper, **K.N. Maloney**

1:55 AGFD **155.** Changes in lipid profile and plasma proteome of streptozotocin-induced diabetic rats fed an amaranth supplemented diet. **A.J. Velarde Salcedo**, A. Barrera Pacheco, A.P. Barba de la Rosa

2:20 Intermission.

2:35 AGFD **156.** Investigation of the antiproliferative constituents of *Podocarpus neriifolius* leading to the isolation of bioactive type-B podolactones and a novel glucoside derivative. **P. Benatrehina**, W. Chen, H. Chai, T.N. Ninh, D.D. Soejarto, J.E. Burdette, L. Rakotondraibe, A.D. Kinghorn

3:00 AGFD **157.** Mechanically robust N-halamine grafted PVA-co-PE membranes with renewable antimicrobial activity. **Y. Si**, Y. Ma, A. Cossu, N. Nitin, G. Sun, D. Wang

3:25 AGFD **158.** Lunasin-enriched products: Effect of Kunitz trypsin and Bowman-Birk protease inhibitors on stability against pepsin-pancreatin hydrolysis and modification of the inflammasomes *in vitro*. **S.J. Price**, P. Pangloli, H. Krishnan, V.P. Dia

3:50 AGFD **159.** Sorghum kafirin: Effect of ultrasonication on its pepsin-pancreatin digestibility and anti-inflammatory effects in lipopolysaccharide-induced THP-1 human macrophages. **A. Sullivan**, P. Pangloli, V.P. Dia

4:15 AGFD **160.** Particle size related bacterial recovery in immunomagnetic separation. **J. Chen**, B. Park

4:40 Concluding Remarks.

Nanocellulose Processing & Analysis

Fundamentals

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Sponsored by CELL, Cosponsored by AGFD

Undergraduate Research Posters

Agricultural & Food Chemistry

Sponsored by CHED, Cosponsored by AGFD‡ and SOCED‡

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

N. P. Seeram, *Organizer*

8:00 - 10:00

38, 40, 47, 49, 51, 53, 55, 57, 59-60, 64, 86-88, 91, 93-95, 98-100, 103, 105, 107-108, 110. See previous listings.

TUESDAY MORNING

Section A

Hilton San Francisco Union Square
Continental Parlor 9

Chemistry & Biological Activities of Phenolic Compounds from Fruits & Vegetables

Mass Spectrometry & Invitro Biological Activities

G. Gattuso, B. Patil, *Organizers*

G. K. Jayaprakasha, *Organizer, Presiding*

G. Williamson, J. Zawistowski, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **161.** Cryo-TOF-SIMS visualization of water-soluble chemicals in plant. D. Aoki, Y. Matsushita, **K. Fukushima**

8:30 AGFD **162.** Towards a comprehensive analysis of condensed tannin structures. **H. Fulcrand**, L. Rouméas, C. Romieu, L. Mouls, J. Brillouet

8:55 AGFD **163.** Chemical composition of flavonoids from selected herbs and their mechanism of inhibition of dipeptidyl peptidase-IV as potential strategy in the management of diabetes. **E.G. Demejia**, A. Bower, M.A. Berhow

9:20 AGFD **164.** Mass spectrometry techniques for metabolomics and tissues imaging of natural products from Lychnophora species, a flavoring agent in the Brazilian traditional spirit. **N. Lopes**

9:45 Intermission.

10:00 AGFD **165.** Nanoencapsulated curcumin demonstrated higher cytotoxicity of colon cancer cells through enhanced bioavailability. G.K. Jayaprakasha, K. Murthy, **B. Patil**

10:25 AGFD **166.** Potential cancer chemopreventive activity of fruit phytochemicals from black chokeberry, goji, and maqui berry botanical dietary supplements. **B. Naman**, J. Li, P. Benatrehina, L. Pan, W. Keller, A. Kinghorn

10:50 AGFD **167.** Expanding human blood metabolomics to the analysis of coenzymes and antioxidants using 1H NMR spectroscopy. **G. Gowda**, D. Raftery

11:15 AGFD **168.** Proanthocyanidins from Chinese Bayberry (*Myrica rubra* Sieb. et Zucc.) leaves regulate lipid metabolism and glucose consumption by activating AMPK pathway in HepG2 cells. **Y. Zhang**, X. Ye, S. Chen

11:40 Concluding Remarks.

Section B

Hilton San Francisco Union Square
Franciscan A

Chemistry of Tree Nuts

A. E. Mitchell, *Organizer, Presiding*

K. Lapsley, *Presiding*

8:00 AGFD **169.** Health effects of tree nuts: Nothing but good news. **J.A. Vinson**

8:25 AGFD **170.** Beyond benzaldehyde: The chemistry of raw, roasted and rancid almonds. **A.E. Mitchell**

8:50 AGFD **171.** Chemical and nutritional characterization of the wrapped cashew. **L.L. Oehrl**

9:15 Intermission.

9:35 AGFD **172.** Comparison of analytical GC-MS techniques for the determination of volatile and semi-volatile compounds in raw and roasted Macadamia nuts *(Macadamia integrifolia)*. **S.J. Toth**

10:00 AGFD **173.** Metabolomics based approach identifies changes in the composition of small molecular weight compounds in the peanut seed after dry-roasting. **C.M. Klevorn**, L.L. Oehrl

Section C

Hilton San Francisco Union Square
Franciscan B

Artisanal Foods

M. H. Tunick, *Organizer*

A. L. Waterhouse, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 AGFD **174.** Chemistry of artisanal cheese. **M.H. Tunick**, S. Doughty

8:50 AGFD **175.** Mexican Cotija cheese: Flavors that keep more than 400 years of tradition. **P.M. Chombo-Morales**

9:15 AGFD **176.** Artisanal and sourdough breads. **B. Klein**, **A.S. Ross**

10:00 Intermission.

10:15 AGFD **177.** Understanding the flavor and quality of honey. **A.E. Mitchell**, A. Harris

11:00 AGFD **178.** Quality and authenticity assessment of extra virgin olive oil. **S. Wang**, D. Garci-aguirre

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

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TUESDAY AFTERNOON

Section A

Hilton San Francisco Union Square
Continental Parlor 9

Chemistry & Biological Activities of Phenolic Compounds from Fruits & Vegetables

Invitro Studies

G. K. Jayaprakasha, B. Patil, *Organizers*

G. Gattuso, *Organizer, Presiding*

J. Kim, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **179.** C- and O-glycosyl flavones in pigmented orange juices: Identification, quantification and evaluation of their influence on antioxidant and cytoprotective activity. **D. Barreca**, E. Bellocco, S. Ficarra, G. Laganà, E. Tellone, A. Galtieri, G. Gattuso

1:30 AGFD **180.** Identification, quantification and mechanism study of potential anti-inflammatory hydroxycinnamic Acid Amides from root bark of *Lycium barbarum*. **S. Wang**, Y. Wang, C. Ho, J. Suh

‡ *Cooperative Cosponsorship*

1:55 AGFD **181.** Evaluation of abiotic environmental conditions on phytochemical and biological activities in Abies koreana. **J. Kim**, D. Kim, E. Park

2:20 AGFD **182.** Bioactive compounds and cellular antioxidant activity of selenized *P. ostreatus* fruiting bodies. **J.A. Carrasco-Gonzalez**, J. Gutierrez-Uribe, S.O. Serna-Saldivar

2:45 Intermission.

3:00 AGFD **183.** Aronia berry: Polyphenols, anti-inflammatory activity, and lipid modulation. **B.W. Bolling**

3:25 AGFD **184.** Cranberry proanthocyaidins: Effects on *Helicobacter pylori* and uropathogenic *Escherichia coli*. **A.B. Howell**

3:50 AGFD **185.** *In vitro* and *in vivo* a-glucosidase inhibition of vitexin and isovitexin. **C. Choo**

4:15 Concluding Remarks.

Section B

Hilton San Francisco Union Square

Franciscan A

Chemistry of Tree Nuts

A. E. Mitchell, *Organizer, Presiding*

K. Lapsley, *Presiding*

1:00 AGFD **186.** Almond and hazelnut are rich in tannins, with varying proportions of bound proanthocyanidin. **B.W. Bolling**

1:25 AGFD **187.** Sensory evolution of rancidity in roasted almonds. L.M. Franklin, **E. King**, **D.M. Chapman**, N. Byrnes, G. Huang, A.E. Mitchell

1:50 AGFD **188.** Walnut: Unique health benefits among the tree nuts. **J.A. Vinson**

2:15 Intermission.

2:35 AGFD **189.** Physical property influence on almond fracture properties and digestibility. **G. Bornhorst**, C. Floyd, Y. Mennah Govela

3:00 AGFD **190.** Advanced life cycle modeling of California almond production systems. E. Marvinney, A. Kendall, **E. Spang**, S. Brodt, F. Shilling, J. Fulton

Section C

Hilton San Francisco Union Square

Franciscan B

General Papers

N. P. Seeram, *Organizer, Presiding*

H. Ma, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **191.** Biodegradable matrix for sustained release of pesticides for crop protection. **T. Pirzada**, A. Salam, N. Burns, R. Mathew, R.H. Guenther, T.L. Sit, M. Byrd, L. Pal, C. Opperman, S.A. Khan

1:30 AGFD **192.** Optimization and validation of 360 pesticides multiresidue method for GC-MS/MS in brown rice, orange and spinach. **J. Lee**, Y. Shin, J. Lee, J. Lee, M. Jung, S. Baek, D. Jeon, H. Yu, X. Yuan, E. Kim, J. Kim

1:55 AGFD **193.** Synthesis and evaluation of natural herbicide, Thaxtomin A and analogous. **N. Esmati**, **J. Bourgault**, A. Reddy Maddirala, P.R. Andreana, **J. Gray**

2:20 AGFD **194.** Development of the simultaneous analytical method for aryloxyphenoxypropionate herbicides and their metabolites in rice and pepper using LC-MS/MS. **J. Lee**, J. Lee, E. Kim, Y. Shin, J. Lee, M. Jung, S. Baek, X. Yuan, D. Jeon, H. Yu, J. Kim

2:45 Intermission.

3:00 AGFD **195.** Development of analytical method for pesticide multi-residues in egg and milk using GC-ECD/NPD. **J. Lee**, J. Lee, Y. Shin, J. Lee, E. Kim, M. Jung, S. Baek, D. Jeon, X. Yuan, H. Yu, J. Kim

3:25 AGFD **196.** Multi-residue screening method for the determination of 380 pesticides in human urine by liquid chromatography-tandem mass spectrometry. **Y. Shin**, J. Lee, E. Kim, J. Lee, M. Jung, S. Baek, H. Kim, J. Kim, M. In, H. Lee, J. Kim

3:50 AGFD **197.** Mosquito larvicidal activity of some isocoumarins. **K.M. Meepagala**, **A. Estep**, **J.J. Becnel**

4:15 AGFD **198.** Potato chips: A simple model for odor image encoding. **M.M. Rochelle**, T. Acree, G. Prevost, C. Maxe

4:40 Concluding Remarks.

Advances in Polysaccharides: Practice & Applications

New Developments in the Industrial Sector

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

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WEDNESDAY MORNING

Section A

Hilton San Francisco Union Square

Continental Parlor 9

Chemistry & Biological Activities of Phenolic Compounds from Fruits & Vegetables

Invivo Studies

G. Gattuso, G. K. Jayaprakasha, B. Patil, *Organizers*

S. Poulose, J. F. Stevens, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **199.** Dietary polyphenols and health: Novel mechanisms of action involving their in vivo metabolites. **D. Del Rio**

8:30 AGFD **200.** Raspberry (poly) phenolics exert bioactivity following *in vivo* digestion. **C. Gill**, C. Latimer, G. McMullan, R. Lawther, G. McDougall, D. Stewart, G. Pereira-Caro, A. Crozier, K. Rotjanapun, I. Rowland

8:55 AGFD **201.** Polyphenol- and PUFA-rich walnuts protect against age-associated cognitive decline through epigenetic modulation. **S. Poulose**, B. Shukitt-Hale

9:20 Intermission.

9:35 AGFD **202.** Mice fed high fat diets supplemented with red, golden or black Arkansas apple peels have reduced weight and differences in gut microbiota. M. Friedman, S. Elkahoui, D. Sturges, G.E. Bartley, C. Levin, **W.H. Yokoyama**

10:00 AGFD **203.** Prenylated flavonoids from hops (*Humulus lupulus)* for treatment of metabolic syndrome. **J.F. Stevens**

10:25 AGFD **204.** Potential effects of flavonoids from breadfruit in prevention of Advanced Glycation End products (AGEs)-induced biological events. J. Lin, **G. Yen**

10:50 Concluding Remarks.

Section B

Hilton San Francisco Union Square

Franciscan A

Bliss Point: Food Satiety & Food Mood Effects

B. Burton-Freeman, I. Edirisinghe, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **205.** Food chemistry, satiety and food intake regulation. **B. Burton-Freeman**

8:35 AGFD **206.** Brain and behavioral responses to fructose vs. glucose. **K.A. Page**

9:05 AGFD **207.** Dynamic relationships between emotion and food perception. **H. Seo**

9:35 AGFD **208.** Is UMAMI, the 5th basic taste, to control satiety? **H. Uneyama**

10:05 AGFD **209.** Appetite regulating hormones and eating behaviors in healthy adults. **N.L. Keim**, S. Krishnan, W.F. Horn, A. Widaman, K. Stanhope, M.G. Witbracht, S.M. Forester, K.D. Laugero, J.W. Newman, M. Van Loan

Section C

Hilton San Francisco Union Square

Franciscan B

General Papers

N. P. Seeram, *Organizer, Presiding*

H. Ma, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **210.** HPAE-PAD Determination of carbohydrates in honey. **M. Aggrawal**, **J. Rohrer**

8:30 AGFD **211.** Stabilization of natural pigments from purple corn pericarp in a beverage model through complex formation with metal ions and polysaccharides. **R. Cortez**, D. Luna, E.G. Demejia

8:55 AGFD **212.** Polycyclic aromatic hydrocarbons in vegetable oils by gas chromatography with SIM mode mass spectrometry. **A.C. Litin**, V. Vega

9:20 AGFD **213.** Simultaneous extraction of gingerols and polysaccharides from ginger (*Zingiber officinale* Roscoe) with ionic liquid-based ultrasonic-assisted extraction. **X. Kou**, Y. Ke, Y. Xie, H. Wang, Y. Su

9:45 Intermission.

10:00 AGFD **214.** Use of reconstituted egg yolk systems to study the roles of plasma and granules in yolk gelation induced by freezing-thawing. **M. Primacella**, T. Wang, N. Acevedo

10:25 AGFD **215.** Designing and optimizing light protection dairy milk packaging. **C.M. Stancik**, D.A. Conner, P. Niedenzu, P. Jernakoff

10:50 AGFD **216.** Improved stability of whey protein fibrils and utility for biomaterial application. **O.G. Jones**, **J. Gilbert**

11:15 AGFD **217.** Withdrawn.

11:40 AGFD **218.** Bioactive compounds present in karela peel extract [*Momordica charantia]:* Potential inhibitors of advanced glycation endproducts (AGEs) and implications in diabetes type 2 patients. **B. Dayal**, M.A. Lea, **V. Dobariya**, P. Bhalala, K. Sahithi, B. Patel, S. Roy, C. Navadia, P. Chauhan, A. Shah, Y. Attoti, P. Antwi

12:05 Concluding Remarks.

Bio-based Gels & Porous Materials

Biopolymer Hydrogels

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Advances in Polysaccharides: Practice & Applications

Novel Biocatalytic & Biopolymeric Approaches

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Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

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WEDNESDAY AFTERNOON

Section A

Hilton San Francisco Union Square

Continental Parlor 9

Chemistry & Biological Activities of Phenolic Compounds from Fruits & Vegetables

Invivo & Human Clinical Trials

G. Gattuso, G. K. Jayaprakasha, B. Patil, *Organizers*

A. Crozier, D. Ghosh, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **219.** Phenolic compounds accumulation in wild and domesticated cladodes from *Opuntia spp.:* Their relation with changes in their metabolism. A. Negre-Salvayre, F. Guéraud, M. Santos Díaz, **A.P. Barba de la Rosa**

1:30 AGFD **220.** Metabolic and microbiome innovations for improving phenolic bioactives for health. **K. Shetty**, D. Sarkar

1:55 AGFD **221.** Absorption, distribution, metabolism and excretion of orange juice flavanones in endurance trained athletes. **A. Crozier**

2:20 AGFD **222.** Safety of cocoa flavanol intake in healthy adults. **J. Ottaviani**

2:45 Intermission.

3:00 AGFD **223.** Polyphenols from fenugreek: Wellness and medicinal uses. **D. Ghosh**

3:25 AGFD **224.** Flavonoids in onion beef soups: Stability, reactivity and potential health benefits. **M. Wang**, Y. Zhao

3:50 AGFD **225.** Effect of phenolic compounds on sugar metabolism: Mechanism of protection against developing type 2 diabetes. **G. Williamson**

4:15 Concluding Remarks.

Section B

Hilton San Francisco Union Square
Franciscan A

Chemistry of Cellulosic Natural Products

S. Chang, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 AGFD **226.** Infrared imaging of cotton fiber bundles and products. **M. Santiago**, D. Hinchliffe, J.E. Rodgers

1:30 AGFD **227.** *In situ* synthesis and application of silver nanoparticles as an antimicrobial agent for cotton fibers. **K.R. Fontenot**, S. Nam, B.D. Condon

1:55 AGFD **228.** Alkaline extraction of residual hemicellulose in dissolving pulp and its properties. **C. Kim**, T. Floyd, T. Treasure, S. Kelley, S. Park

2:20 Intermission.

2:35 AGFD **229.** Multifunctional chitosan-based nanocoatings: Stopping oxygen and fire with renewable materials. **J.C. Grunlan**

3:00 AGFD **230.** Anti-flammable properties of casein with phosphorus and nitrogen containing flame retardants on cotton by layer-by-layer self assisted coating processing. **S. Chang**, B.D. Condon, J. Smith

Section C

Hilton San Francisco Union Square
Franciscan B

General Papers

N. P. Seeram, *Organizer, Presiding*

H. Ma, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **231.** Non-targeted chemometric detection of adulterated olive oils by flow injection mass spectrometric fingerprints. **D. Lijuan**, W. Lu, L.L. Yu

1:30 AGFD **232.** Characterization of uranium exposure in sheep grazing near abandon uranium mines on the Navajo reservation. **A.R. Lister**, J.C. Ingram

1:55 AGFD **233.** U.S. Dairy Forage Research Center (DFRC) condensed tannin NMR database. **W. Zeller**, P. Schatz

2:20 AGFD **234.** Detecting and distinguishing among type 1 and type 2 Shiga toxins in human serum. **C.J. Silva**, M.L. Erickson-Beltran, C.B. Skinner, S.A. Patfield, X. He

2:45 Intermission.

3:00 AGFD **235.** Optical probe for the detection of a spoilage indicator in shrimp. **R.A. Federico Perez**, Z. Xue

3:25 AGFD **236.** Fate and transport of electronic waste degradation products in soil and water. **S. Moller**, A. Chaparadza

3:50 AGFD **237.** Magnetic-Encoded fluorescent multifunctional nanoprobes for multiplex pathogenic bacteria assay. **E. Song**

4:15 AGFD **238.** Normpack-The Swedish code for food packaging materials since year 1981. **K. Salmen**

4:35 AGFD **239.** Lycopene a panacea for sustainable man power for agricultural production in Nigeria: Determination of lycopene from water melon (*Citrullus lanatus)*. **S. Okonkwo**

5:00 Concluding Remarks.

Bio-based Gels & Porous Materials

Biopolymer Organogels

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Advances in Resource Recovery & Conservation in Water Systems

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Advances in Polysaccharides: Practice & Applications

Novel Materials & Methodologies

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Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

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THURSDAY MORNING

Section A

Hilton San Francisco Union Square
Continental Parlor 9

General Papers

N. P. Seeram, *Organizer, Presiding*

W. Liu, H. Ma, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **240.** Enhancement of catalytic activity and stability of crude Laccase extract in Silica Sol-Gel. **J. Gill**, V. Orsat, S. Kermasha

8:30 AGFD **241.** Stabilization and protection of retinyl palmitate in policosanol oleogels. **Y. Tian**, N. Acevedo

8:55 AGFD **242.** Rationale behind the near-ideal catalysis of *Candida antarctica* Lipase A (CAL-A) for highly concentrating ω-3 polyunsaturated fatty acids into monoacylglycerols. **Z. Guo**

9:20 AGFD **243.** Molecularly imprinted polymers based colorimetric-sers dual biosensor for the detection of atrazine in foods. **B. Zhao**, X. Lu

9:45 Intermission.

10:00 AGFD **244.** Chemical defence and novel biosynthetic pathways of phytoalexins in crucifers. **Q. To**, M. Pedras

10:25 AGFD **245.** RNA-seq reveals insight into the molecular mechanism of biocontol yeast antagonistic against aflatoxigenic *Aspergillus flavus*. **S.T. Hua**

10:50 AGFD **246.** Here come the potato shock troops: Investigating temporal resistance of potato tubers to microbial infection using antibacterial activity and metabolite profiling of wound-healing tissue extracts from contrasting cultivars. **K. Dastmalchi**, M.E. Perez Rodriguez, A. Mychak, J. Linn, A. Janakiraman, R.E. Stark

11:15 AGFD **247.** Disaggregation of amyloid beta peptides by ginnalin A, a glucitol-core containing gallotannin from red maple (*Acer rubrum):* Biophysical, bioanalytical, and cytotoxicity studies. X. Wang, H. Ma, Z. Li, **F. Zhou**, N.P. Seeram

11:40 Concluding Remarks.

Section B

Hilton San Francisco Union Square
Franciscan A

Synthetic Biology in Food & Agriculture

N. Nitin, J. Talbert, R. S. Tiwari, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:10 AGFD **248.** Computational identification of new ingredients. **C. Anderson**

8:35 AGFD **249.** Emerging organism engineering industry. **S. Reisinger**

9:00 AGFD **250.** Human design of food and crops. **J. Medford**

9:25 AGFD **251.** Securing the global food web. **M. Koeris**

9:50 AGFD **252.** Recombinant bacteriophages serve as sensitive bacterial recognition elements. **T.C. Hinkley**, S. Nugen

10:15 AGFD **253.** FDA's approach to the safety assessment and regulation of food ingredients. **R. Merker**

10:40 Discussion.

Section C

Hilton San Francisco Union Square
Franciscan B

Coffee & Cocoa Products

M. Granvogl, M. C. Qian, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 AGFD **254.** Molecularizing the taste of cocoa (*Theobroma cacao)*. **T.D. Stark**, T. Hofmann

8:35 AGFD **255.** Influence of caffeine-polyphenol-melanoidin interactions on the bitter taste perception of coffee beverages. **O. Frank**, T. Hofmann

9:05 Intermission.

9:25 AGFD **256.** Characterization of key odorants of dark chocolate by means of the sensomics approach. C. Seyfried, **M. Granvogl**

9:55 AGFD **257.** New insight into the role of flavour precursors upon coffee roasting. **T. Davidek**, L. Poisson, F. Mestdagh, I. Blank

Bio-based Gels & Porous Materials

Aero-, Cryo- & Xerogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Resource Recovery & Conservation in Water Systems

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Advances in Polysaccharides: Practice & Applications

New Functional Materials

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Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

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THURSDAY AFTERNOON

Section A

Hilton San Francisco Union Square
Continental Parlor 9

General Papers

N. P. Seeram, *Organizer, Presiding*

H. Ma, *Presiding*

1:00 Introductory Remarks.

1:05 AGFD **258.** Influence of pre-fermentation apple juice clarification on the chemistry of hard cider. **S. Ma**, A. Neilson, G. Peck, S.F. Okeefe, K. Hurley, A. Sandbrook, A. Stewart

1:30 AGFD **259.** Encapsulation of policosanol enriched sugarcane wax for food supplement application. **S. Sittiwanichai**, S. Boonyarattanakalin, S. Jarussophon, I. Sramala, W. Pinket, P. Pongwan, K. Kasemwong

1:55 AGFD **260.** Oxidation of olive oil and canola oil: Applications in organic chemistry. L. Callen, **Z. Van Scyoc**, **D. Morelli**, **M. Glick**

2:20 Intermission.

2:35 AGFD **261.** Investigation into the chemical properties of traditional and so-called drug-store varieties of pipe tobaccos and the impact of the US FDA's Substantial Equivalence (SE) rules on the continued marketability of those products. **J.H. Lauterbach**

3:00 AGFD **262.** Significance of cooking oil to bioaccessibility of DDTs and PBDEs in raw and cooked fish. X. Mi, Y. Su, **L. Bao**, E. Zeng

3:25 AGFD **263.** Hydrogen peroxide quantitation in complex matrices – A fluorimetric method using Amplex Red. **S. Chakraborty**, A.L. Hill, G. Shirsekar, A. Afzal, G. Wang, D. Mackey, P. Bonello

3:50 AGFD **264.** Dye-Sensitized solar cell for STEM learning. **P. Hill**

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4:15 AGFD **265.** Chiral monoterpene profiles of aromatic white wines. **M. Song**, C. Fuentes, A. Loos, E. Tomasino

4:40 Concluding Remarks.

Section B

Hilton San Francisco Union Square
Franciscan A

Coffee & Cocoa Products

M. Granvogl, M. C. Qian, *Organizers*, *Presiding*

1:00 AGFD **266.** Role of roasting conditions in the formation of bioactive chemicals in coffee. J. Moon, M. Kamiyama, **T. Shibamoto**

1:30 AGFD **267.** Trends in coffee and cocoa products and the complexity of described formulations. **P. Son**, V.A. Biehl, E.M. Altizer, A. Windhof, R.B. McWhirter

2:00 AGFD **268.** Withdrawn.

2:30 Intermission.

2:50 AGFD **269.** FTIR analysis of gasses emitted during roasting coffee. **S. Amanuel**, P. Catravas, J.D. Kehlbeck

3:20 AGFD **270.** Identification of coffee constituents with beneficial effects on cholesterol metabolism. **V. Somoza**, W. Hoffmann

3:50 Concluding Remarks.

Bio-based Gels & Porous Materials

Open-Porous Carbon Materials

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Advances in Resource Recovery & Conservation in Water Systems

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Advances in Polysaccharides: Practice & Applications

Preparation, Characterization & Applications

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Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

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AGRO

Division of Agrochemicals

S. Jackson, *Program Chair*

SUNDAY MORNING

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

SUNDAY AFTERNOON

Hollyweird Chemistry

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Contaminants of Emerging Concern in Natural & Engineered Systems

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MONDAY MORNING

Hollyweird Chemistry

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Contaminants of Emerging Concern in Natural & Engineered Systems

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MONDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

WEDNESDAY AFTERNOON

Contaminants in Urban & Coastal Estuarine Ecosystems

Advanced Analytical Techniques to Assess Chemical Profiles

Sponsored by ENVR, Cosponsored by AGRO

WEDNESDAY EVENING

Contaminants in Urban & Coastal Estuarine Ecosystems

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Contaminants of Emerging Concern in Natural & Engineered Systems

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THURSDAY MORNING

Contaminants in Urban & Coastal Estuarine Ecosystems

Environmental Processes Affecting Chemical Availability & Toxicity

Sponsored by ENVR, Cosponsored by AGRO

THURSDAY AFTERNOON

Contaminants in Urban & Coastal Estuarine Ecosystems

Temporal & Spatial Assessment of Persistent-Bioaccumulative Chemicals in Coastal & Urban Waters

Sponsored by ENVR, Cosponsored by AGRO

ANYL

Division of Analytical Chemistry

L. Baker and K. Phinney, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation (see *ENVR*, Sun, Mon, Wed)

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies (see *ENFL*, Tue, Wed)

Contaminants of Emerging Concern in Natural & Engineered Systems (see *ENVR, Sun,* Mon, Wed)

Frontiers in Glycoanalytics (see *CELL*, Wed, Thu)

Nanocellulose Processing & Analysis (see *CELL*, Sun, Mon)

Separation of Macromolecules & Particulates (see *POLY,* Sun)

SOCIAL EVENTS:

Reception, 5:00 PM: Tue

SUNDAY MORNING

Section A

Hilton San Francisco Union Square
Union Square 14

Synthesis & Characterization of Materials for Energy Applications

Enabling Concepts for Energy Materials Design

Cosponsored by CATL

J. Rodriguez Lopez, K. J. Stevenson, *Organizers*

D. R. Rolison, *Organizer, Presiding*

V. Augustyn, *Presiding*

8:30 ANYL **1.** Thin-Film pair distribution analyses of energy-storage materials in device-ready 3D electrodes. **D.R. Rolison**, M.D. Donakowski, J.M. Wallace, M.B. Sassin, K.W. Chapman, J.F. Parker, J.W. Long, C.N. Chervin, I.R. Pala, A.N. Mansour

9:00 ANYL **2.** Synthesis and characterization of solvated transition metal oxides for electrochemical energy storage. R. Wang, J. Mitchell, W. Lo, **V. Augustyn**

9:30 ANYL **3.** Decreasing impedance and increasing capacity in solid state electrochemical cells through architectural optimization. **E.D. Wachsman**

10:00 Intermission.

10:30 ANYL **4.** First principles optimization of novel solar cell materials. **E.A. Carter**

11:00 ANYL **5.** Interfacing nanomaterials for solar-to-fuel conversion. P. Yang, **D. Kim**

11:30 ANYL **6.** Probing intrinsic stability of complex metal halides: A transition from hybrid to all inorganic perovskite solar cells. **P.A. Troshin**, L.A. Frolova, A. Akbulatov, S. Luchkin, K.J. Stevenson

Section B

Hilton San Francisco Union Square
Franciscan D

Advances in Separations

J. L. Maclachlan, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **7.** Simultaneous estimation of ketorolac tromethamine and phenylephrine hydrochloride in artificial aqueous humor. **F.B. Tandel**, R. Trivedi

8:25 ANYL **8.** Aqueous normal phase chromatography: A new approach to complex sample analysis. **J.J. Pesek**, M. Matyska

8:45 ANYL **9.** Rapid determination of cocamidopropyl betaine impurities in cosmetic products by core-shell HILIC-MS/MS. **P.G. Wang**, W. Zhou

9:05 ANYL **10.** Adaption of Ehrlich's Reagent to a HPLC post-column reaction system for the quantification of limonoid glucosides. **A.P. Breksa**, D.E. King, A.M. Vilches

9:25 ANYL **11.** New HPLC method development workflow by leveraging state-of-the-art software. **L. Wang**

9:45 ANYL **12.** Integration of out-of-plane optical fiber for multipoint detection in microfluidic platforms and using fiber tunneling mode for particle/cell counting, velocimetry and size discrimination. **D. Ediriweera**, J. Sadeghi, C.T. Culbertson

10:05 Intermission.

10:15 ANYL **13.** Investigating the gas chromatography separation properties of azulene- and naphthalene-modified polysiloxanes. **M. Jackson**, C.M. Garner

10:35 ANYL **14.** Screening and on-site identification of accelerants for arson investigations. **J.L. Maclachlan**, J.N. Driscoll

10:55 ANYL **15.** Polymer-based gas chromatography microcolumns. **J.J. Hinman**, K.S. Suslick

11:15 ANYL **16.** Alternative to commercial instrumentation. **S. Abbott**, D. Faries, R. Taylor

11:35 Concluding Remarks.

Section C

Hilton San Francisco Union Square
Union Square 17/18

New Analytical Advances in Accelerator Mass Spectrometry (AMS)

Financially supported by National Electrostatics Corporation

B. A. Buchholz, *Organizer, Presiding*

8:30 ANYL **17.** PIMS progress. **S. Freeman**, R. Shanks, C. McIntyre, G. Gaubert

8:50 ANYL **18.** Chemi-ionization in the Cs sputter ion source: Selective ionization for AMS. **J.S. Vogel**

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

9:10 ANYL **19.** Developing AMS hyphenations with analytical instruments for atmospheric aerosol characterization. **G. Salazar**, K. Agrios, S. Szidat

9:30 Intermission.

9:45 ANYL **20.** Streamlining analyses of atmospheric carbonaceous aerosols: Determining the sources of fires in Indonesia. **E. Wiggins**, **G. dos Santos**, **C. Czimczik**, J. Randerson

10:05 ANYL **21.** Plasma oxidation prior to accelerator mass spectrometry radiocarbon dating. **K.L. Steelman**

10:25 ANYL **22.** Compound specific radiocarbon analyses at NOSAMS: Unlocking ocean and lake chronologies one molecule at a time. **A.P. McNichol**, L. Xu, W. Longo, A. Gagnon, M. Roberts, S. Shah Walter, B. Longworth, Y. Huang

10:45 ANYL **23.** Macromolecular isolation and purification in AMS. **B.A. Buchholz**, K.L. Spalding, R. Dreier, I. Maze, B.J. Mailloux, S.A. Carratt, L.S. Van WInkle, T. Ognibene, E. Kuhn, N. Hum, N. Etminan, G.G. Loots

Section D

Hilton San Francisco Union Square

Franciscan C

Coherent Multidimensional Spectroscopy in Materials Science

Cosponsored by PHYS

W. Zhao, *Organizer, Presiding*

A. T. Krummel, *Presiding*

8:00 ANYL **24.** Multiresonant coherent multidimensional spectroscopy of MoS2. **J.C. Wright**, K. Czech, B. Thompson

8:30 ANYL **25.** Fast electronic dynamics in 2D spectra of PbS quantum dots. S.D. Park, D. Baranov, J. Ryu, **D.M. Jonas**

9:00 ANYL **26.** Two dimensional electronic spectroscopy of methyl ammonium lead halide perovskite nanocrystals. **G.S. Engel**, L. Wang

9:30 ANYL **27.** Exciton dynamics in transition metal dichalcogenide monolayers revealed by two-dimensional electronic spectroscopy. **L. Guo**, D.M. Monahan, G.R. Fleming

10:00 Intermission.

10:15 ANYL **28.** Resolution and selectivity: Major advantages of coherent 3D spectroscopy over coherent 2D spectroscopy. **P. Chen**

10:45 ANYL **29.** Pushing signal-to-noise ratio toward the detector limit in multidimensional spectroscopy. **N. Ge**

11:15 ANYL **30.** Two-dimensional electronic Stark spectroscopy. **J.P. Ogilvie**, A. Loukianov, A. Niedringhaus, B. Berg

Section E

Hilton San Francisco Union Square

Union Square 19/20

Analytical Neuroscience

Financially supported by Pittcon

A. C. Michael, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ANYL **31.** Microfabricated and mass spectrometry tools for In Vivo monitoring of neurochemicals. **R. Kennedy**

9:05 ANYL **32.** Aptamer field-effect transistors as neurochemical sensors to monitor neurotransmitters *in vivo*. **N. Nakatsuka**, K. Yang, Y. Rim, X. Xu, J. Abendroth, C. Zhao, Y. Yang, M. Stojanovic, P.S. Weiss, A.M. Andrews

9:35 ANYL **33.** Extraction and detection of neurotransmitters and anesthetic drug in-vivo based on polymeric ionic liquids. **X. Zhou**, Y. Zhang, G. Shi

10:05 Intermission.

10:20 ANYL **34.** Faster neurochemical measurements using continuous on-line microdialysis: Towards microdialysis 2.0. **M.G. Boutelle**, I.C. Samper, A. Leong, M.L. Rogers, S. Gowers, A.M. Nightingale, X. Niu

10:50 ANYL **35.** Some considerations on limitations and opportunities in making measurements in living tissue. **S.G. Weber**, Y. Ou

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Nanocellulose Processing & Analysis

Novel Processes

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

Separation of Macromolecules & Particulates

Sponsored by POLY, Cosponsored by ANYL, COLL and PMSE

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Sponsored by ENVR, Cosponsored by ANYL

SUNDAY AFTERNOON

Section A

Hilton San Francisco Union Square

Union Square 14

Synthesis & Characterization of Materials for Energy Applications

In Operando & Surface Sensitive Analysis

Cosponsored by PHYS

J. Rodriguez Lopez, K. J. Stevenson, *Organizers*

D. R. Rolison, *Organizer, Presiding*

J. E. Pemberton, *Presiding*

1:30 ANYL **36.** Generation and evolution of materials in the anode Solid Electrolyte Interphase (SEI) of lithium ion batteries. **B.L. Lucht**

2:00 ANYL **37.** Application of local probes of structure to characterize supercapacitor and battery function. A. Forse, C. Merlet, K.J. Griffith, P.K. Allan, **C.P. Grey**

2:30 ANYL **38.** Understanding and design of core-shell architectures for battery electrodes based on complex oxides. **J. Cabana**

3:00 Intermission.

3:30 ANYL **39.** Organic semiconductor interfaces in optoelectronic devices: Undesirable chemistry galore! **J.E. Pemberton**, L. Sang, K.E. Watts, T. Nguyen, E.L. Ratcliff

4:00 ANYL **40.** Chemomechanically mediated processes in energy devices. **H. Tavassol**

4:30 ANYL **41.** Dendrites and pits: Untangling the complex behavior of lithium metal anodes through operando video microscopy. K.N. Wood, E. Kazyak, A.F. Chadwick, J. Zhang, K. Thornton, **N.P. Dasgupta**

Section B

Hilton San Francisco Union Square

Franciscan D

Advances in Separations

J. L. Maclachlan, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **42.** Ionic liquid surfactants in cationic polyacrylamide gel electrophoresis protein separation. **P. Vidanapathirana**, F. Hasan, K. Mussio, N. Siraj, A. Grove, I.M. Warner

1:25 ANYL **43.** Stirred-electromembrane extraction at low voltages as a novel microextraction technique for analysis of basic drugs. **K.M. Ara**

1:45 ANYL **44.** Microchip electrophoresis separation of pre-term birth biomarkers in a 3D printed device. **M.J. Beauchamp**, H. Gong, G.P. Nordin, A.T. Woolley

2:05 ANYL **45.** Capillary electrophoresis coupled with micro free flow electrophoresis for high speed comprehensive two dimensional analysis of peptides. **A.C. Johnson**, M. Bowser

2:25 ANYL **46.** Three-phase direct immersion in-tube microextraction coupled with capillary electrophoresis. J. Choi, Y. Choi, **D. Chung**

2:45 Intermission.

2:55 ANYL **47.** Affinity extraction of DNA for sepsis diagnosis using on-chip monoliths. **R. Knob**, A. Woolley

3:15 ANYL **48.** SFE and preparative SFC with mass directed collection as beneficial tools in the workflow for natural products isolations from complex mixtures. **J.P. McCauley**

3:35 ANYL **49.** Determination of sodium nitrite in peanut paste baits by ion chromatography. **B.G. Abbo**, S.F. Volker

3:55 ANYL **50.** Evaluation and comparison of pulsed-electromembrane extraction and electromembrane extraction techniques for the analysis of fluoxetine and olanzapine in biological fluids. **K.M. Ara**

4:15 Concluding Remarks.

Section C

Hilton San Francisco Union Square

Union Square 17/18

New Analytical Advances in Accelerator Mass Spectrometry (AMS)

Financially supported by National Electrostatics Corporation

B. A. Buchholz, *Organizer, Presiding*

1:30 ANYL **51.** Technological developments for BioAMS applications. **T. Ognibene**

1:50 ANYL **52.** Ultrasensitive Bio-AMS applications for safe and environmentally relevant clinical studies of high molecular weight polycyclic aromatic hydrocarbon pharmacokinetics. **E. Madeen**

2:10 ANYL **53.** Coupled accelerator mass spectrometer-mass spectrometer analysis of biomolecules. **B. Stewart**

2:30 ANYL **54.** Use of accelerator mass spectrometry for precision medicine applications in cancer therapy. **P.T. Henderson**, T. Scharadin, M. Zimmermann, T. Ognibene, R. de Vere White, K. Turteltaub, G. Cimino, E. Kim, A. Yu, B. Jonas, C. Pan

2:50 Intermission.

3:05 ANYL **55.** Combined use of HRMS and combustion AMS for simultaneous metabolite quantification and identification. E.V. Duijn, **W. Vaes**

3:25 ANYL **56.** AMS enabled clinical studies in GSK: Past, present and future. **G.C. Young**

3:45 ANYL **57.** Stategies for efficient metabolite characterization by UPLC + AMS. H. Lee, S. La, **S. Dueker**

4:05 ANYL **58.** Automation of 14C-labeled, biological-sample measurements by cavity ring-down spectroscopy and comparison to accelerator mass spectrometry. **A. McCartt**, T. Ognibene, G. Bench, K. Turteltaub

Section D

Hilton San Francisco Union Square

Franciscan C

Coherent Multidimensional Spectroscopy in Materials Science

Cosponsored by PHYS

W. Zhao, *Organizer*

P. B. Petersen, M. C. Thielges, *Presiding*

1:00 ANYL **59.** Dynamics of functionalized alkyl monolayers on gold: Two dimensional infrared experiments and molecular dynamics simulations. **M.D. Fayer**

1:30 ANYL **60.** What can be learned from high-order spectroscopies? The hidden dynamics of rate-exchange. J.R. Darvin, H. Kaur, **M.A. Berg**

2:00 ANYL **61.** Development of femtosecond multidimensional spectroscopies to probe vibronic couplings in molecules and materials. J.D. Gaynor, Z. Fox, M. Balasubramanian, **M.H. Khalil**

‡ *Cooperative Cosponsorship*

2:30 ANYL **62.** High-throughput 2D IR spectroscopy platform yields insights into solvent dynamics in solution mixtures. **A.T. Krummel**, K. Tracy, C. Carver

3:00 Intermission.

3:15 ANYL **63.** Charge separation in 2D crystal heterostructures. **J. Zheng**

3:45 ANYL **64.** Conformations and dynamics of protein molecular recognition via 2D IR spectroscopy. **M.C. Thielges**, S. Ramos, A. Le Sueur, R. Horness

4:15 ANYL **65.** Investigating lipid membrane interfaces with 2D IR spectroscopy. **C. Baiz**, J. Flanagan, M. Valentine, S. Edington

Section E

Hilton San Francisco Union Square
Union Square 19/20

Analytical Neuroscience

Financially supported by Pittcon

A. C. Michael, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ANYL **66.** Single- and sub- cellular observation of acetylcholine neurotransmission with a nanopipet electrode. **M. Shen**

2:05 ANYL **67.** Voltammetric investigation of serotonin's roles in depression. **P. Hashemi**

2:35 ANYL **68.** Probing *in vivo* neurochemistry by microdialysis sampling coupled to mass spectrometry. **L. Li**

3:05 Intermission.

3:20 ANYL **69.** Mathematical model to optimize electroenzymatic microbiosensors for the monitoring of glutamate signaling in the brain. **M. Clay**, H.G. Monbouquette

3:50 ANYL **70.** Unraveling the neurochemistry of 'chemobrain'. **M.A. Johnson**, S. Kaplan, T. Field, R. Gerhinger

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodolgies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Nanocellulose Processing & Analysis

Process Parameters

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Separation of Macromolecules & Particulates

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Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Sponsored by ENVR, Cosponsored by ANYL

SUNDAY EVENING

Section A

Moscone Center
West Hall

Analytical Division Poster Session

K. Phinney, *Organizer*

7:00 - 9:00

ANYL **71.** Quantitative detection of carbazole and halogenated carbazoles in human blood samples. **J. She**

ANYL **72.** Effects of ozone on representative molecular components in epicuticular waxes of leaves: Oleanolic and ferulic acid. **C. Smith**, M. Riches, T. Kochar, D.P. Soulsby, T.L. Longin

ANYL **73.** Development of highly sensitive personal use colorimetric fumigant sensors. **P. Tang**, G. Sun

ANYL **74.** Characterization of short-chain dicarboxylic acids in the infrared region using Beer's Law. **N.Q. Vu**, C. Cooper, P.K. Hudson

ANYL **75.** Determination of airborne mercury using Ag-nanoparticles assisted TXRF. **S. Boettger**, D. Rosenberg, M. Busker, W. Jansen, U.E. Fittschen

ANYL **76.** Evaluating suspect screening and non-targeted analysis approaches using a collaborative research trial at the US EPA. **A.J. Williams**, A. McEachran, E.M. Ulrich, J. Sobus, A. Richard, C. Grulke

ANYL **77.** Mass-spectrometry based structure identification of "known-unknowns" using the EPA's CompTox dashboard. **A. McEachran**, A.J. Williams

ANYL **78.** Trace anion determinations using inline calibration and an electrolytic water purifier. **T. Christison**, D. Khor, J. Rohrer

ANYL **79.** Analysis of fluoride and pH, in Utah waters, beverages and dental products. **P.J. Iles**, **S. Moore**, A. Abbinanti, J. Morris, K. Robbins, L. Dalby, R. Holcomb, N.R. Bastian, L.D. Giddings, M. Alvarez, R.V. Valcarce

ANYL **80.** Effects of ozone on resveratrol and quercetin: Phytochemicals in grape berry skins. **T. Rogoff**, A. Telfer-Radzat, T. Kochar, D.P. Soulsby, T.L. Longin

ANYL **81.** Cormorant AGE's: When old isn't based on pentosidine concentrations in tissues. **R.S. Stahl**, B. Dorr

ANYL **82.** Investigation of inorganic anions in indoor airborne particular matter during SoCal wildfire season. **H. Zhu**, Y. Liu

ANYL **83.** Quantification of VOCs emitted from cut and uncut grass. **L. Leti**

ANYL **84.** Evolution of the equilibrium vapor pressures of 1,4-bis (phenylethynyl) benzene (DEB) through the hydrogenation process. **E. Sangalang**, **H. Sharma**, G. Cairns, C. Saw, W. McLean II, R.S. Maxwell, L. Dinh

ANYL **85.** Fluorogenic probe for rapid detection of fluoride in water. **S. Bae**

ANYL **86.** Investigation of the sequential flow analysis and the use of nitrate reductase and for the determination of nitrate in sea water and salt water aquaria. **P.J. Iles**, A. Pabon, R. Kochambilli, H. Hauritz, A. Villa, R. Holcomb, M. Alvarez, N.R. Bastian, L.D. Giddings, R.V. Valcarce

ANYL **87.** Continued identification of pharmaceuticals in Utah's Jordan River. **N. Elmore**, P.J. Iles, L.D. Giddings, N.R. Bastian, R. Holcomb, M. Alvarez, R.V. Valcarce, B. Sanders, H. Hsieh, M. Asadian, A. Samani, A. Mineer

ANYL **88.** Investigation of selected metals in soil samples exposed to agricultural and automobile activities in Macedonia, Greece using inductively coupled plasma-optical emission spectrometry. **V. Topalidis**, A. Harris, G.S. Benipal, C. Douvris

ANYL **89.** Monitoring of trace level arsenic in the environmental waters using ZIF-8. **D. Parajuli**, K. Sue, A. Takahashi, T. Kawamoto

ANYL **90.** Development of a novel CE-XRF system for elemental speciation. **I.M. Tyssebotn**, A. Fittschen, U.E. Fittschen

ANYL **91.** Photocatalytic degradation of common pharmaceuticals for disposal. **L.A. Tom**, O. Beale, M. Kalala, E. Juliano, M. Botts

ANYL **92.** Quantification of uranium in soil and sediment from Cameron, AZ. **B.N. Dalton**, J.C. Ingram

ANYL **93.** Visualization of surface adsorption properties of trace metals by rice husks using LA-ICP-MS. **R. Ellerby**, D. Alexander, D.D. Amarasiriwardena

ANYL **94.** Flower-like CuO as electrochemical sensor for thiobencarb detection. **C. Su**, C. Lee, H. Chiu

ANYL **95.** Development of simultaneous analytical method for parent compound and its metabolites of pesticide in livestock products. **S. Yang**, J. Park, H. Choi

ANYL **96.** Perfluorinated bonded phase as a separation medium in high performance liquid chromatography: Evaluation of properties and applications. **T. Nguyen**, J. Topete, **V. Truong**, D. Hong, S. Jarman, T. Pham, C. Pham, T. Mo

ANYL **97.** Determination of polyphenols in mesquite pod flour extracts by HPLC-UV and LC-MS. **T. Nguyen**, J. Topete, **V. Truong**, S. Jarman, D. Hong, T. Pham, C. Pham, T. Mo

ANYL **98.** Diversity, antimicrobial activity and chemical fingerprinting of marine actinomycetes. **R. Kashfi**

ANYL **99.** Rapid screening method for selenium containing dietary supplements. **T. Hanley**, K. Kubachka, S. Kern

ANYL **100.** Matrix extension and multi-laboratory validation of the U.S. Food and Drug Administration method EAM 4.10 to include arsenic speciation in wine. **R.A. Wilson**, C.K. Tanabe, H. Hopfer, S.E. Ebeler, J. Nelson, S. Conklin, K. Kubachka

ANYL **101.** Development of method by UFLC-DAD for identification of the prostaglandin cloprostenol sodium in veterinary pharmaceuticals. **A.M. Miranda**, M.V. de Moura

ANYL **102.** X-ray fluorescence elemental imaging, and micro analysis of plant tissue samples. **U.E. Fittschen**, R. Hoehner, W. Tramel, A. Fittschen, H. Kunz

ANYL **103.** Determination of Sudan I and of a newly synthesized Sudan III positional isomer in the color additive D&C Red No. 17 using high-performance liquid chromatography. A. Weisz, **I.C. James**, C. Tae, C.D. Ridge, Y. Ito

ANYL **104.** Investigation of tissue level distribution of essential and toxic metals in corn seeds from contaminated mining area using LA-ICP-MS. **S. Gaiss**, D. Alexander, F. Wu, D.D. Amarasiriwardena

ANYL **105.** Analysis application in jaboticaba fruit. **J. Guido**

ANYL **106.** Chemotaxonomy of poplar and sourwood honey. **V. Rizzi**, E.B. Grimley, K.D. Sienerth

ANYL **107.** Withdrawn.

ANYL **108.** Bioavailability of methylmercury in rice cereal and fish. **G. Nicholas**, W. Cui

ANYL **109.** Metabolomic profiling of three representative food diets using ion chromatography with high resolution Orbitrap mass spectrometry. **T. Christison**, R. Kiyonami, R. Tautenhaum, J. Rohrer

ANYL **110.** Analytical- and preparative-scale isolation of oleandrin from *Nerium oleander* using microwave-assisted extraction coupled with purification using supported-metal ion solid phase extraction resins. **L.M. Jablonksi**, D.B. Green

ANYL **111.** Interactions of the cell penetrating peptide TAT with model membranes using Scanning electron microscopy, differential scanning calorimetry, and infrared techniques. **N. Phambu**, B.M. Almarwani, A. Sunda-Meya

ANYL **112.** Withdrawn.

ANYL **113.** Glycan microarray-based screening for substrate specificity of sialyltransferase. **H. Heo**, C. Kim, J. Seo, H.J. Cha

ANYL **114.** Electrospray mass spectrometry using an organosiloxane polymer. **M.T. Dulay**, R.N. Zare

ANYL **115.** Gradient chromatofocusing: Multiple buffer components for the separation of prolactin isoforms. **A. Gobburi**, H. Jogiraju, I. Tirak, J. Tirak, D. Anderson

ANYL **116.** Photonic crystal microplate for high performance multi-anion recognition. **Y. Liu**, C. Yu, J. Lv, C. Wei

ANYL **117.** Development and validation of a sensitive ultra-performance liquid chromatographic method with tandem mass spectrometry for quantification of doxorubicin in human plasma. **M. Semreen**, H. Al-niss, M. Mousa, R. El-Awady

ANYL **118.** Red-NIR perylene-based fluorescent dyes for detection of DNA G-quadruplexes. **L. Huang**, **G.H. Aryal**, K.W. Hunter

ANYL **119.** Detection of heterogeneity of mAb and corresponding Antibody Drug Conjugates (ADCs) by size exclusion chromatography and its orthogonal and complimentary modes. **A. Chakrabarti**

ANYL **120.** Which is worse? Hookah consumption or cigarette smoking, a preliminary study on toxicity. **R.T. Saadawi**, T. Hanley, A.A. Clutterbuck, M. Nashu, J. Landero

ANYL **121.** Faster and improved ease-of-use citrate and phosphate assays of pharmaceutical products. **H. Yang**

ANYL **122.** Analysis of Cu(II)-mediated dityrosine cross-linking of amyloid-beta in-vitro and in-vivo by MALDI MS. **A. Kelley**, G. Perry, S.B. Bach

ANYL **123.** Evaluation of human NAD(P)H:Quinone Oxidoreductase Isozyme-1 (HNQO1) expression and activity in several human ovarian carcinoma cell monolayers. **M. Jackson**, R.L. McCarley

ANYL **124.** Fabrication and application of microfluidic devices for safety test of cosmetics. **T. Tian**

ANYL **125.** Sensitive analysis of cancer biomarkers using nonlinear multi-photon laser wave mixing detector interfaced to micellar capillary electrophoresis. **J. Liang**

ANYL **126.** Trichloroacetic acid improves MS signal and separation in determination of tobramycin in M9 bacterial medium by LC-MS/MS. **L. Huang**, J. Haagensen, D. Verotta, V. Cheah, A. Spormann, F. Aweeka, K. Yang

ANYL **127.** Study of mouse enamel proteins by imaging mass spectrometry. **M. Colley**, Y.P. Chun, S.B. Bach

ANYL **128.** Using Reversed-Phase High Performance Liquid Chromatography Mass Spectrometry (RP-HPLC-MS) for domain-specific free thiol variant characterization of an IgG1. **Y. Cheng**, M. Chen, Y. Chen, C. Yu, T.Y. Zhang, B. Burgess

ANYL **129.** Withdrawn.

ANYL **130.** Direct electrochemical sensing of hydrogen sulfide. **J. Hall**, M. Schoenfisch

ANYL **131.** Multiplexed quantitation of cancerous tRNA biomarkers by capillary electrophoresis. H. Chen, Y. Huang, W. Lin, **P. Chang**

ANYL **132.** Analyzing global metabolite variation based on mutations in the tricarboxylic acid cycle of *Escherichia Coli* using high resolution mass spectrometry. **E.D. Tague**, J. Wen, H.F. Castro, E. Fozo, S.R. Campagna

ANYL **133.** Microwave-assisted synthesis of SBD-F derivatives for the HPLC-FLD determination of four biological aminothiols. **M.B. Blayney**, D.B. Green

ANYL **134.** Spectroscopic studies on CTAB-lysozyme-Vitamin C. N. Barbier, J. Lacoste, **H. Yan**

ANYL **135.** Hydrogen deuterium exchange mass spectrometry analysis of lipid free apoliporpotein A-I dimer. C. Topbas, C. Baleanu Gogonea, I. Choucair, H. Alamri, J. Didonato, J. Smith, S. Hazen, **V. Gogonea**

ANYL **136.** Ruthenium-modified sensitive NO sensors: Quantifying nitric oxide in the pathobiology of cystic fibrosis. **T. Bose**

ANYL **137.** Fundamental studies of ferriprotoporphyrin polymerization on electrode surfaces for H2S detection. **J.A. Bennett**, S. Simpson, E. Zurek

ANYL **138.** Differentiation of species using aptamers binding to unknown targets in organism. **Y. Jeong**, B. Lee, H. Han, M. Gu

ANYL **139.** Investigating the Intracellular Fate of NaYF4:Yb,Er@NaYF4 conjugated siRNA in HeLa Cells. **M. Shahrukh**

ANYL **140.** Preparative HPLC methods with type-C columns. **J. Topete**, M. Matyska, J.J. Pesek

ANYL **141.** Determination of folic acid concentration in tick samples with cogent DH columns. **J. Topete**, J. Chen, J. Zhong, M. Matyska, J.J. Pesek

ANYL **142.** Enzyme kinetics studies to guide mathematical modeling of microdialysis sampling to predict *in situ* biochemistry. **J. Klucher**, J.A. Stenken

ANYL **143.** Monitoring rapid reactions with ambient pressure ionization mass spectrometry. **E. Jansson**, R.N. Zare

ANYL **144.** Probing intracellular micro-environments through spectrally resolved STORM. **S. Moon**, R. Yan, S. Kenny, Y. Shyu, W. Li, K. Xu

ANYL **145.** Droplets microfluidic platform for high throughput enzyme screening. **X. Diefenbach**

ANYL **146.** Poly-adenine tailed DNA probe based self-assembly monolayer engineering for electrochemical biosensors. **L. Li**, Y. Wen, J. Meng, L. Wang, Q. Xu, W. Liang, **G. Liu**

ANYL **147.** Characterization of corticotropin (ACTH) products by Liquid Chromatography High Resolution Mass Spectrometry (LC-HRMS). **K. Zeng**, C. Sommers, D. Keire

ANYL **148.** Imaging the distribution of selective GABAA receptor modulators in the asthmatic lung using MALDI assisted mass spectrometry. **M. Guthrie**

ANYL **149.** Single-Molecule fluorescence imaging of mismatched and modified oligonucleotide hybridization. M.W. Manhart, E.M. Peterson, **J.M. Harris**

ANYL **150.** Surface sandwich SPR biosensing platforms for tau proteins in plasma sample. **H. Lee**, S. Kim

ANYL **151.** Analysis of formation and recognition of three G-quadruplexes in c-myb proto-oncogene. **F. Li**, J. Zhou, **G. Yuan**, **J. Li**

ANYL **152.** Exploring the formation and high affinity recognition of miR-1587 G-quadruplex by spectroscopy. W. Tan, J. Zhou, J. Li, **G. Yuan**

ANYL **153.** Facile electrochemical melting of surface-bound DNA with minimal electrostatic screening. **D. Ho**, N. Le, A. Chin, W. Hetrick, R. West

ANYL **154.** DNA aptamers that bind with high affinity to hydroxyapatite. **J. Florek**, A.E. Gerdon

ANYL **155.** Electrochemical oxidation of albendazole on electrode surface: Chromatographic determination of drug metabolites. **A.M. Mugweru**, Z. Mazzochette, G.N. Kamau

ANYL **156.** TIR-Enhanced Raman system for sensitive and selective identification of volatile organic compounds. **C.J. Taylor**, A. Niemz, K.J. Park, R. Dodson, C. Wu, H. Lu, P. Rentzepis, P. Koonath

ANYL **157.** Magnesium ribbon-templated microfluidic device and a diffusion limited titration. C.F. Monson, **J. Barney**

ANYL **158.** Water-soluble conjugated polymers for the detection and inhibition of protein aggregation. **R. Chai**, **Y. Zhan**, **C. Xing**

ANYL **159.** Withdrawn.

ANYL **160.** Folic acid- and transferrin-functionalized gold nanoparticles for targeted delivery and controlled release of anti-cancer drug Gemcitabine. **T. Santiago**, K. Kurzatkowska, M.R. Hepel

ANYL **161.** Controlled release of anti-leukemia drugs azacitidine and decitabine monitored using SERS. **M. Smith**, M.R. Hepel

ANYL **162.** ROS induced by FRET between upconversion nanoparticle and photosensitizer for targeted photodynamic cancer therapy. **W. Hou**, W. Tan

ANYL **163.** Characterization of phospholipid bilayers in copolymer belted nanodiscs by electrokinetic chromatography. **W. Penny**, C.P. Palmer

ANYL **164.** Label-Free detection of small molecule-membrane protein binding kinetics using self-assembled nano-oscillators. **G. Ma**, X. Shan, S. Wang, N. Tao

ANYL **165.** Single gold nanoparticle gas sensing based on photothermal effect. **X. Li**, L. Zhang

ANYL **166.** Super-resolution optical imaging of interaction between metal nanoparticles based on microsphere. **B. Hou**, L. Zhang

ANYL **167.** Study of single Pt nanoparticle collision: Against electrocatalytic activity on a Pd UME. **C. Park**

ANYL **168.** Detection of copper single nanoparticle collision on gold ultramicroelectrode by electrocatalytic amplification. **K. Kim**

ANYL **169.** Synthesis and characterization of conductive polymer hydrogels and the investigation of their application as a biosensor hybrid for the detection of catechol. **V. Grebe**, E. Castillo, B. Palys, J. Widera

ANYL **170.** Adsorption, decomposition, and surface-assisted laser desorption/ionization of asphaltenes using transition metal oxide nanoparticles. **L. Barnes**, **J.R. Yount**, K.A. Reyes, K.E. King, P.M. Kirkconnell, H. Hamilton, S.S. Ward, A. Olaitan, K.S. Molek

ANYL **171.** Biosensing based on ordered gold nanoshell arrays with plasmonic tunability. **W. Qian**

ANYL **172.** Towards paper based assays with intinsically labeled oligonucleotide probes on QDs for detetction of selective hybridization. **A. Shahmuradyan**, U.J. Krull

ANYL **173.** Multiplexed resonance energy transfer nucleic acid hybridization assay using a single form of upconversion nanoparticle as donor and three quantum dots as acceptors. **S. Doughan**, U.J. Krull

ANYL **174.** Liquid biopsy of type-III mutant EGFR in exosomes by using CD63 specific aptamer modified magnetic nanoparticles and qPCR. **Z. Li**, B. Li, L. He, N. He

ANYL **175.** Towards a paper-based oligonucleotide assay for point-of-care detection of disease using immobilized quantum dots as donors in fluorescence resonance energy transfer. **K. Malhotra**, O. Noor, T. Vimalarajah, U.J. Krull

ANYL **176.** Synthesis of functioned multiwalled carbon nanotubes and the application in analysis of small biomolecules by matrix assisted laser desorption/ionization mass spectrometry. **J. Meng**, C. Shi, L. Li, C. Deng

ANYL **177.** Thermoresponsive nanoparticle agglomeration reversibility in salt: Dependence on graft density. **T. Vasicek**, L. Vaz, J.A. Stenken

ANYL **178.** Assessing the electrochemical response of microcontact-printed silver nanogrids utilizing cyclic voltammetry. **W.C. Sanders**, P.J. Iles, J.S. Smith, M. Alvarez, N.R. Bastian, R. Holcomb, L.D. Giddings, R.V. Valcarce, A.C. Lines, J. Meyers, G. Johnson, C. Page, K. Salisbury, C.F. Thompson, D. Young

ANYL **179.** Rechargeable Zn–air battery! architecture, design, and synthesis strategies that go beyond Li-Ion. M.N. Vila, C.N. Chervin, J.F. Parker, J. Ko, P.A. DeSario, J.W. Long, **D.R. Rolison**

ANYL **180.** Asymmetric chemical modification of Photosystem I enabling orientationally-selective deposition on gold electrodes. **C. Bryant**, E.A. Gizzie, D.E. Cliffel

ANYL **181.** Fuel cell catalyst formation by simultaneous reduction of platinum (IV) and graphene oxide. **T.E. Kusumadjaja**, W. Zhou

ANYL **182.** Chemometric evaluation of multifeedstock biodiesel diesel blended fuels. **A.M. Hupp**, M. Flood, C. Mary, M. Comiskey

ANYL **183.** Modifying carbon electrodes to behave like precious metals. J.C. Lytle, **G. Kamm**, A.D. McGovern, J.F. Parker, M.D. Donakowski, D.R. Rolison, J.W. Long

ANYL **184.** Sensitive and selective detection of explosives by nonlinear optical laser wave-mixing spectroscopy. **J. Pradel**, A. Jackson, G. Varnau, W.G. Tong

ANYL **185.** Soil survey for southwest Louisiana and its potential forensic applications. **J. Higginbotham**, S. Bonilla, C. Becktold, A. Tizeno, P. Spencer

ANYL **186.** Bath salts analyzed via HPLC. **M. Makhanov**, A. Lopez, J.J. Pesek, M. Matyska

ANYL **187.** Biological sex determination via bioaffinity-based fingerprint analysis. **C. Huynh**, E. Brunelle, J. Agudelo, L. McGoldrick, L. Halámková, J. Halamek

ANYL **188.** Fingerprint analysis: Chemical assays for the identification of biological sex. **E. Brunelle**, C. Huynh, A.M. Le, L. Halámková, K. Wingfield, J. Agudelo, L. McGoldrick, J. Halamek

ANYL **189.** Withdrawn.

ANYL **190.** GC-MS/MS analyses of biological samples in support of developmental toxic effects of exposure to sarin in rats via multiple routes. **J.M. McGuire**, L. Lumley, M. Busch, L. Wright, P. Demond

ANYL **191.** Selective and sensitive capture of pathogens on imprinted Sol-gel polymers. **M.T. Dulay**, N. Zaman, R.N. Zare

ANYL **192.** Total vaporization of derivatization reagent for in situ headspace derivatization solid phase microextraction. L. Perry, **J. Yu**

ANYL **193.** Forensic science research and development programs at the National Institute of Justice: Opportunities in analytical chemistry. **G.J. Dutton**

ANYL **194.** Forensic quantitative analysis of opiates in post-mortem blood and brain: Application of DLLME-LC/MS/MS. **M.A. Hunt**, **W.J. Morrison**, L.D. Muir, A. Tully, W.W. Jenkins, L.E. Lowe, **J.E. Owens**

ANYL **195.** GC-FID Method for the forensic discrimination of lipstick residues. **B. Esterlen**, **B.J. Bellott**

ANYL **196.** Probing the use of a UHPLC Whelk-O1 chiral stationary phase in eUHPSFC-MS for chiral/achiral analysis of naturally occurring cannabinoids. **M.J. Wilcox**, G. Mazzoccanti, O.H. Ismail, A. Ciogli, C. Villani, F. Gasparrini, S. Anderson

ANYL **197.** Smartphone-assisted colorimetric analysis of Mn in stainless steel. **C. Huang**, B. Lum, Y. Liu

ANYL **198.** 2D IR spectroscopy study of 13C-natural abundant vibrational transition in Mn(CO)5Br. **Y. Fan**, J.P. Wang

‡ *Cooperative Cosponsorship*

ANYL **199.** Nanohydroxyapatite-Nanocellulose composites as bioactive scaffolds for applications in bone tissue regeneration. **S. Laboy**, C.I. Rivera, E. Nicolau

ANYL **200.** Development of methods for kinetic analysis of templated and untemplated calcium phosphate mineralization. **K. Luarasi**, **K. Meserve**, **J. Miech**, A.E. Gerdon

ANYL **201.** Effect of energy per atom (E/n) in Ar gas cluster ion beam (GCIB, Arn+) and O2+ cosputter. **S. Wang**, J. Shyue

ANYL **202.** Withdrawn.

ANYL **203.** Electro-photodynamic visualization of singlet oxygen induced by zinc porphyrin modified microchip in aqueous media. C. Zheng, H. Cui, Y. Wan, **S. Deng**

ANYL **204.** Synthesis and characterization of meso-tetrakis(2-fluoro-4-methoxyphenyl)porphyrin and its copper(II) and cadmium(II) derivatives. **A. Adeyemo**

ANYL **205.** Solution spectral characteristics of metallophthalocyanine. **A. Adeyemo**

ANYL **206.** Meso-tetrakis(2-chloro-3quinolyl) porphyrin and its water-soluble derivative meso-tetrakis(2-chloro-4-sulfonato-3-quinolyl)porphyrin. **A. Adeyemo**

ANYL **207.** Ligand exchange reactions involving copper(I) thiamine complexes and water-soluble porphyrin, 5,10,15,20-tetrakis(2,4-dimethyl-5-sulfonatophenyl)porphyrin. **A. Adeyemo**

ANYL **208.** Synthesis and characterization of three isomeric porphyrins for Photodynamic Therapy of tumor (PDT). **A. Adeyemo**

ANYL **209.** Preparation and characterization of a new photosensitizer and its metal derivatives: Potential anticancer drugs. **A. Adeyemo**

ANYL **210.** Synthesis and characterization of porphyrins for photodynamic therapy of tumor (PDT). **A. Adeyemo**

ANYL **211.** Withdrawn.

ANYL **212.** Introducing analytical chemistry to Navajo undergraduates through field research: Uranium exposure of sheep grazing near abandoned mines. **J.C. Ingram**, D.K. Robinson

ANYL **213.** Development of novel paper- and fabric-based microfluidic fuel cells and batteries. **F.A. Gomez**, A. Avoundjian, A. Mendez, C. Tang, F. Bernal, S. Valiulis, R. Ortiz, V. Galvan, K. Domalaon, M. Gonzalez

ANYL **214.** From sample to answer: A low-cost disposable cartridge for epidemic detection on site based on 3D printing technology. **N. He**, H. Chen, Y. Deng

ANYL **215.** Polyvinyl alcohol modified porous graphitic carbon stationary phase for hydrophilic interaction liquid chromatography. **H. Yanjie**, Z. Feifang, Y. Bingcheng

ANYL **216.** Withdrawn.

ANYL **217.** PCR-free ligase cyclic reaction for SNP detection of KRAS mutation with attomole sensitivity. **J. Kim**

ANYL **218.** Development of NIRS calibration models for pharmaceutical quality control analysis. **J. Feng Baez**, J.E. Mercado-Adrover, V. Cárdenas, R.J. Romanach

ANYL **219.** Self-assembly of the cephalopod structural protein reflectin. **K. Naughton**, L. Phan, E. Leung, R. Kautz, Q. Lin, Y. van Dyke, B. Marmiroli, B. Sartori, A. Arvai, S. Li, M. Pique, M. Naeim, J. Kerr, M. Aquino, V. Roberts, E. Getzoff, C. Zhu, S. Bernstorff, A.A. Gorodetsky

ANYL **220.** Detection of low level nitrate in seawater by combining Ag nanoparticles and Au electrode. **K. Fajerwerg**, E. Lebon Tailhades, P. Fau, M. Kahn, M. Comtat, P. Temple Boyer, B. Dubreuil, **P. Behra**

ANYL **221.** Use of Graphene-Oxide (GO) for both aptamer screening and fluorescence aptasensor in the detection of whole avian viruses. **S. Kim**, Y. Kwon, J. Lee, M. Kim, H. Cho, C. Song, M. Gu

ANYL **222.** Withdrawn.a

ANYL **223.** Withdrawn.

ANYL **224.** Withdrawn.

ANYL **225.** Antenna-Coupled Plasmonic Nanowire Endoscope (ACPNE) for label-free remote sensing in single live-cells. **S. Kim**, Y. Zhu, R. Yan

ANYL **226.** Withdrawn.

ANYL **227.** Photolysis of a Zn(II)-nitriliotriacetate cage in AOT/isooctane reverse micelles. **C.N. Beuning**, T. Paryani, N.E. Barkley, P. Basa, R.L. Cole, N.E. Levinger, S.C. Burdette, D.C. Crans

ANYL **228.** Way to go green! Evaluation of different analytical SFC systems. **M. Goel**, A. Kumar

ANYL **229.** Inhibition of MYC-induced lipogenesis prevents renal cell carcinoma initiation and progression. A. Gouw, **K. Margulis**, D. Sullivan, G. Toal, L. Eberlin, C.V. Dang, R.N. Zare, D. Felsher

ANYL **230.** Superfast two-phase reactions in microdroplets without the use of phase transfer catalyst. **X. Yan**, H. Cheng, S. Banerjee, R.N. Zare

ANYL **231.** Withdrawn.

ANYL **232.** Development of impidimetric aptasensor devices for the analytical determination of inorganic arsenic. **E. Nicolau**, K. Vega

ANYL **233.** Human *in vivo* protein corona formed onto liposomes in ovarian carcinoma patients: From characterization to potential clinical utilization. **M. Hadjidemetriou**, K. Kostarelos

ANYL **234.** Ratiometric resonance synchronous spectroscopy for material characterizations. **D. Zhang**

ANYL **235.** Development of a biomineralization strategy for surface modification of single glass nanopore: Versatile nanopores for fluoresence observation and electrochemical chiral sensing. **A. Zhu**, **S. Cao**, G. Shi

ANYL **236.** Asymptomatic diagnosis of Huanglongbing disease using metalloporphyrin functionalized single-walled carbon nanotubes sensor arrays. **H. Wang**, P. Ramnani, T. Pham, C. Villarreal, G. Liu, A.K. Mulchandani

ANYL **237.** Nanostructured superhydrophobic organic semiconductor films enable sub-zeptomole level molecular sensing in surface-enhanced Raman spectroscopy. **G. Demirel**, H. Usta, A. Facchetti

ANYL **238.** Withdrawn.

ANYL **239.** Non-fouling SERS substrate for detect the cationic fluorescent tag from human blood solution. **T. Wen**

ANYL **240.** Determination of second hyperpolarizability with computational Raman activities and identification of DOVE signatures for selected molecules. **W. Zhao**

MONDAY MORNING

Section A

Hilton San Francisco Union Square

Union Square 14

Synthesis & Characterization of Materials for Energy Applications

Enabling Concepts for Energy Materials Design

Cosponsored by CATL

J. Rodriguez Lopez, D. R. Rolison, *Organizers*

K. J. Stevenson, *Organizer, Presiding*

A. Kolpak, *Presiding*

8:30 ANYL **241.** Tuning the electrocatalytic activity of perovskite oxides for water oxidation and oxygen reduction by active site variation. **K.J. Stevenson**, W. Hardin, R. Forslund, C. Alexander, K.P. Johnston

9:00 ANYL **242.** Role of interface structure and stoichiometry on water splitting in oxide photo- and electrocatalysts. **A. Kolpak**

9:30 ANYL **243.** Measurement strategies and challenges for the study of heterogeneous water oxidation electrocatalysts. **S.W. Boettcher**, M. Burke-Stevens, L. Enman

10:00 Intermission.

10:30 ANYL **244.** First-principles comparative study of Li, Na and Mg intercalation compounds. **A. Van der Ven**, M. Radin, J. Vinckeviciute

11:00 ANYL **245.** Reflection on the performance defining properties induced by the positive electrode – Electrolyte interface chemistry. **G.G. Amatucci**, N. Pereira, F. Badway, N. Faenza

11:30 ANYL **246.** Ab initio band-diagram framework for the development of cation intercalation charge storage materials. M. Young, A.M. Holder, S.M. George, **C. Musgrave**

Section B

Hilton San Francisco Union Square

Franciscan D

ACS Award in Chromatography: Symposium in honor of Robert T. Kennedy

L. Huang, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 ANYL **247.** Capillary LC with sub-2 micron particles: Effects of column packing conditions on column morphology and efficiency. **J.W. Jorgenson**, J. Godinho, A. Reising, U. Tallarek

9:10 ANYL **248.** Phosphoproteomics of fertilization. E. Peuchen, P. Huber, K. Dubiak, L. Sun, **N.J. Dovichi**

9:40 ANYL **249.** Toward resolving large isomeric glycans. **M.V. Novotny**

10:10 Intermission.

10:25 ANYL **250.** Charting protein-protein interactions using Cross-Linking Mass Spectrometry (XL-MS). C. Yu, C. Gutierrez, X. Wang, E. Novitsky, S.D. Rychnovsky, **L. Huang**

10:55 ANYL **251. Award Address** (ACS Award in Chromatography sponsored by MilliporeSigma). High-speed electrophoresis as an enabling technology for protein analysis, screening, and sensing. R. Kennedy

Section C

Hilton San Francisco Union Square

Union Square 17/18

Chemical Forensics

Investigations of Alleged Use & Source Attribution of Chemical Weapons

Cosponsored by CHAL and PRES

R. Foster, C. Fraga, J. J. Moran, *Organizers*

J. R. Cort, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ANYL **252.** Influence of analytical chemistry on multilateral diplomacy and chemical disarmament. **J.E. Forman**

8:25 ANYL **253.** Analysis in support of investigations of alleged use. **H. Gregg**

8:45 ANYL **254.** Analysis of biomedical samples of victims after exposure to sarin or sulfur mustard. **P. Vanninen**, U. Hakala, M. Söderström, O. Kostiainen, M. Rapinoja

9:10 ANYL **255.** Phosphatidylglycerol chlorohydrins as potential biomarkers for chlorine gas exposure. P. Hemström, A. Larsson, L. Elfsmark, **C. Astot**

9:35 ANYL **256.** DHS S&T chemical forensics program. **R. Bull**

9:50 Intermission.

10:05 ANYL **257.** Chemical forensics for sourcing sarin. **C. Fraga**

10:30 ANYL **258.** Small-scale production of chemical warfare agents for chemical attribution signature determination. **S. Hok**

10:55 ANYL **259.** Chemical forensics using multivariate data analysis of chemical attribution signatures from production of chemical warfare agents. **K. Höjer Holmgren**, D. Wiktelius, R. Magnusson, S. Lindberg, A. Larsson, R. Norlin

11:20 ANYL **260.** Chemical attribution of chemical warfare agents for forensic purposes. D. Noort, **M.J. Van der Schans**

11:40 ANYL **261.** Chemical threat agent attribution signature studies by Isotope Ratio Mass Spectrometry technology (IRMS). **K. Hoang**, L. Hoffland, G. Hondrogiannis, S. Ostazeski

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Section D

Hilton San Francisco Union Square
Franciscan C

Coherent Multidimensional Spectroscopy in Materials Science

Cosponsored by PHYS

W. Zhao, *Organizer*

J. M. Anna, E. Harel, *Presiding*

8:00 ANYL **262.** Multidimensional spectroscopy of conical intersections by broadband x-ray pulses. **S. Mukamel**

8:30 ANYL **263.** *In situ* probe of interfacial electric field, catalyst structure and dynamics at electrode/ liquid interfaces by time-resolved vibration sum-frequency generation spectroscopy. **T. Lian**

9:00 ANYL **264.** Dynamic intermediates in singlet fission observed with ultrafast infrared spectroscopy. C. Grieco, G. Doucette, **J.B. Asbury**

9:30 ANYL **265.** Ultrafast vibrational energy delocalization in graphdiyne. **J.P. Wang**

10:00 Intermission.

10:15 ANYL **266.** Energy transfer in solar cells made from semiconducting carbon nanotubes studied using 2D white-light spectroscopy. **M.T. Zanni**

10:45 ANYL **267.** Exploring energy transfer in photosynthetic light harvesting. **G. Schlau-Cohen**

11:15 ANYL **268.** Two-Dimensional electronic spectroscopy of Photosystem I and light harvesting chromophores. **J.M. Anna**

Section E

Hilton San Francisco Union Square
Union Square 19/20

Biomedical Advances in Cancer Detection & Therapeutics Using Advanced Analytical Techniques

C. Burton, Y. Ma, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ANYL **269.** Surface-Enhanced Raman scattering biosensor for cancer protein biomarker detection. **N. Wu**

8:55 ANYL **270.** Nanoscale tools for biomarker discovery: The emerging role of nanoparticle biomolecule corona. **M. Hadjidemetriou**, K. Kostarelos

9:15 ANYL **271.** Investigation of biomarkers to screen for prostate cancer in urine using gas chromatography/mass spectrometry. **A. Siegel**, A. Daneshkhah, J. Munshi, T.A. Gardner, M. Agarwal

9:35 ANYL **272.** Mass spectrometric imaging of prostate biopsy samples: Cancer margin assessment from the distribution of small metabolites and lipids. **S. Banerjee**, R. Zare, R. Tibshirani, C. Kunder, R. Nolley, R. Fan, J. Brooks, G. Sonn

9:55 Intermission.

10:10 ANYL **273.** *In vitro* detection of miR-21 target using a nucleic acid self-quenching smart probe. **S.A. Oladepo**

10:30 ANYL **274.** In vitro manipulation of stimuli-responsive liposomal contents release potentially activated by overexpressed hNQO1 in cancer cells. **H.H. Nguyen**

10:50 ANYL **275.** Evaluating the transfection efficacy of spherical nucleic acid coated upconverting nanoparticles in cells for in vitro imaging and daignostics. **H. Najib**

11:10 ANYL **276.** Current trends in cancer biomarker discovery using urinary metabolomics: Achievements and new challenges. **C. Burton**, Y. Ma

11:30 Concluding Remarks.

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Nanocellulose Processing & Analysis Properties

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Sponsored by ENVR, Cosponsored by ANYL

MONDAY AFTERNOON

Section A

Hilton San Francisco Union Square
Union Square 14

Synthesis & Characterization of Materials for Energy Applications

In Operando & Surface Sensitive Analysis

Cosponsored by CATL

D. R. Rolison, K. J. Stevenson, *Organizers*

J. Rodriguez Lopez, *Organizer, Presiding*

H. D. Abruna, *Presiding*

1:30 ANYL **277.** Versatile in situ chemical imaging of alkali ion reactivity at battery interfaces. **J. Rodriguez Lopez**, Z.J. Barton, J. Hui, M. Burgess

2:00 ANYL **278.** Near- and far-field IR spectroscopy of the Si electrode/organic electrolyte interface. **R. Kostecki**, A. Jarry, M. Ayache, H.A. Bechtel, M.C. Martin

2:30 ANYL **279.** Capturing chemical dynamics at the buried electrode-electrolyte interface by in situ imaging mass spectrometry. J. Yu, Y. Zhou, Z. Zhu, **X. Yu**

3:00 Intermission.

3:30 ANYL **280.** Operando methods for the characterization of energy materials. **H.D. Abruna**

4:00 ANYL **281.** Near-Ambient Pressure X-ray Photoelectron spectroscopy for *in situ* and *in operando* studies of electrocatalytic materials. **E. Savinova**

4:30 ANYL **282.** Design consideration for regenerative electrodes for energy storage application. **S. Mukerjee**, S. Ghoshal, J. Li, Q. Jia

Section B

Hilton San Francisco Union Square
Franciscan D

ACS Award in Analytical Chemistry: Symposium in honor of Donald F. Hunt

J. R. Yates, *Organizer, Presiding*

1:00 ANYL **283.** Uniform field ion mobility QTOF MS and in-source ion activation for protein structural studies. **R.T. Kurulugama**, G. Stafford, J.D. Eschweiler, B.T. Ruotolo, J. Fjeldsted

1:45 ANYL **284.** Intrasurgical diagnosis of human brain tumor tissue and surgical margin characterization by DESI-MS. **R.G. Cooks**, C. Alfaro, A. Jarmusch, V. Pirro, Z. Baird, E. Hattab, A. Cohen-Gadol

2:30 ANYL **285.** Investigating aberrant glycosylation in cancer using mass spectrometry: Insight for cancer immunotherapy design. **S. Malaker**

3:15 ANYL **286.** Mapping dynamic protein interaction landscapes in *Saccharomyces cerevisiae* using a novel whole network enrichment approach. **J.R. Yates**, B. Stein, D. Calzolari, M. Lavallée-Adam

4:00 ANYL **287. Award Address** (ACS Award in Analytical Chemistry sponsored by Battelle Memorial Institute). Instrumentation and methods for the identification and sequence analysis of (a) intact proteins on a chromatograpic timescale and (2) tumor specific peptides for immunotherapy of cancer. **D.F. Hunt**

Section C

Hilton San Francisco Union Square
Union Square 17/18

Chemical Forensics

Chemical Attribution Signatures of Illicit Drugs & Toxic Chemicals

Cosponsored by CHAL and PRES

J. R. Cort, R. Foster, J. J. Moran, *Organizers*

C. Fraga, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ANYL **288.** Changes in illicit cocaine hydrochloride processing identified and revealed through multivariate analysis. **J. Mallette**, J. Casale, J. Jordan

1:35 ANYL **289.** Detection of marijuana varieties based on chemical signatures extracted from sample headspace. A. McDaniel, J. Velez, F. Liu, J. Sweet, **C.C. Yu**

2:00 ANYL **290.** Impurity profiling of methamphetamine synthesized from clandestine methylamine. **J.L. Brown**, S. Toske

2:25 ANYL **291.** Multivariate statistical analysis of orthogonal mass spectral data for the identification and route attribution of 3-methylfentanyl. B.P. Mayer, C.A. Valdez, P. Spackman, **A.M. Williams**

2:50 Intermission.

3:10 ANYL **292.** Source attribution of fentanyl through impurity and stable isotope and trace element profiling. **A. Bennett**, P. Hough, **D. Noort**, N.J. Cooper, D. Alkema, A. Patel, J. Riches

3:35 ANYL **293.** Signature profiling of illicit fentanyl and fentanyl-related seizures for tactical and strategic intelligence. **J. Casale**, J. Mallette

4:00 ANYL **294.** Forensic profiling of amanita mushrooms by high resolution LC-MS. **D. Jansson**, A. Wolterink, C. Astot

4:20 ANYL **295.** Anionic, isotopic, and elemental signatures for forensic source attribution of cyanides. **N.S. Mirjankar**, C. Fraga, A.J. Carman, J.J. Moran

4:40 ANYL **296.** Chemical attribution signatures of cyanogen chloride from commercial sources. **D.B. Cullinan**

Section D

Hilton San Francisco Union Square
Franciscan C

Coherent Multidimensional Spectroscopy in Materials Science

Cosponsored by PHYS

W. Zhao, *Organizer*

T. R. Calhoun, G. Schlau-Cohen, *Presiding*

1:00 ANYL **297.** Using multi-order Time Correlation Functions (TCFs) to elucidate biomolecular reaction pathways from microsecond single-molecule fluorescence experiments. **A.H. Marcus**

1:30 ANYL **298.** Interferometric 2D-SFG spectroscopy of molecular catalysts on TiO2 surfaces. H. Vanselous, A.M. Stingel, **P.B. Petersen**

2:00 ANYL **299.** Quantum coherence selective 2D Raman spectroscopy to probe electron-phonon interactions in hybrid systems. **E. Harel**, A. Spencer, W. Hutson

2:30 ANYL **300.** Time-resolving solid-state solvation using small-molecule dopants in glassy polymer hosts. **M. Delor**, B. Cotts, D. McCarthy, N.S. Ginsberg

3:00 Intermission.

3:15 ANYL **301.** Transient absorption microscopy reveals amphotericin B's mechanism of action. **T.R. Calhoun**, K. Higgins

3:45 ANYL **302.** Optical resonance imaging: An optical analog to MRI with sub-diffraction-limited capabilities. **M.A. Allodi**, R.J. Mazukski, P.D. Dahlberg, J.P. Otto, H. Davis, G.S. Engel

4:15 ANYL **303.** Bandgap inhomogeneity from 2D spectra *vs.* size dispersion from TEM in PbSe quantum dots. **D. Baranov**, S.D. Park, J. Ryu, D.M. Jonas

Section E

Hilton San Francisco Union Square
Union Square 19/20

Biomedical Advances in Cancer Detection & Therapeutics Using Advanced Analytical Techniques

C. Burton, Y. Ma, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 ANYL **304.** Detection of exosomes using fluorescence detection based on competitive hybridization with aptamer. **L. He**, B. Li, Z. Li, P. Xiao, **N. He**

1:55 ANYL **305.** Biosynthesized nanoclusters and supramolecular complexes as scaffolds for multimodal cancer bio-imaging. **X. Wang**

2:15 ANYL **306.** Flotation immunoassay: Masking the signal from free reporters in sandwich immunoassays. **H. Chen**, A. Hagstrom, J. Kim, G. Garvey, A. Paterson, F. Ruiz-Ruiz, B. Raja, U. Strych, M.A. Rito Palomares, K. Kourentzi, J. Conrad, R. Atmar, R.C. Willson

‡ *Cooperative Cosponsorship*

2:35 ANYL **307.** Droplet microfluidic platform for the determination of single-cell lactate release and [18F] fluorodeoxyglucose uptake. **A. Mongersun**, D. Sengupta, P. Asuri, G. Pratx, P. Abbyad

2:55 Intermission.

3:10 ANYL **308.** Biomedical applications of nanoGUMBOS. **N. Bhattarai**, M. Chen, I.M. Warner

3:30 ANYL **309.** Laser-Driven droplet PCR reactions in multiplexed format for gene expression studies. S.S. Dixit, E. Hall, G. Abraham, B. Guo, Z. Ao, R.J. Cote, R. Datar, **G.W. Faris**

3:50 ANYL **310.** Immobilization of circulating tumor cells via polyelectrolyte multilayers allows for free-floating cell visualization and drug screening. **J.I. Andorko**, K.R. Chakrabarti, P. Zheng, S.S. Martin, C. Jewell

4:10 Concluding Remarks.

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

Nanocellulose Processing & Analysis

Fundamentals

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences

Sponsored by ENVR, Cosponsored by ANYL and CHED

Undergraduate Research Posters

Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

L. A. Baker, K. Phinney, *Organizers*

8:00 - 10:00

20, 42, 73, 90, 104, 106, 108, 133, 144, 172, 175, 183-185, 187, 189. See previous listings.

377, 447, 458, 475. See subsequent listings.

TUESDAY MORNING

Section A

Hilton San Francisco Union Square
Union Square 14

Synthesis & Characterization of Materials for Energy Applications

Fundamental & Molecular Models for Advanced Energy Materials

Cosponsored by CATL

J. Rodriguez Lopez, K. J. Stevenson, *Organizers*

D. R. Rolison, *Organizer, Presiding*

S. Brock, *Presiding*

8:30 ANYL **311.** Identification of carbon-encapsulated iron nanoparticles as active species in non-precious metal oxygen reduction catalysts. **A.A. Gewirth**, J. Varnell, A. DiAscro

9:00 ANYL **312.** Electrocatalytic small-molecule transformations using well-defined multilayer films of discrete molecular catalysts. **C.C. McCrory**

9:30 ANYL **313.** Cationic, anionic & electronic disorder on perovskite oxide surface for (electro)catalysis. **W. Chueh**

10:00 Intermission.

10:30 ANYL **314.** Tuning catalytic activity in bimetallic transition metal phosphide nanoparticles via composition control. D. Li, D. Liyanage, S. Mutinda, **S. Brock**

11:00 ANYL **315.** Electrocatalyst design and development for the Oxygen Evolution Reaction (OER) and the electro-reduction of CO2. **T.F. Jaramillo**

11:30 ANYL **316.** Studying the kinetics of electrochemical reactions on ruthenia-coated carbon electrodes. **J.C. Lytle**, G. Kamm, A.D. McGovern, J.F. Parker, M.D. Donakowski, D.R. Rolison, J.W. Long

Section B

Hilton San Francisco Union Square
Franciscan D

Metamorphosis of Supercritical Fluid Chromatography to Chromatographic Systems Using Carbon Dioxide

S. J. Olesik, A. Tarafder, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ANYL **317.** Overcoming major hurdles against the adoption of achiral SFC. **L. Taylor**, M. Ashraf-Khorassani

8:35 ANYL **318.** Separation of polar biological molecules using enhanced-fluidity liquid chromatography. **S.J. Olesik**, R. Bennett, Y. Wang

9:05 ANYL **319.** UHPSFC-MS; The final piece in the analyst's toolbox? . **J.J. Langley**

9:35 ANYL **320.** Fast and high throughput analysis in pharmaceutical process research and development using carbon dioxide based eluents. **C.J. Welch**, K. Zawatzky, E.L. Regalado

10:05 Intermission.

10:20 ANYL **321.** Modeling solvent gradient behavior in SFC. **A. Tarafder**, J.F. Hill

10:50 ANYL **322.** New insights in modern SFC-MS for the analysis of complex samples and biological matrices. **A. Grand-Guillaume-Perrenoud**, A. Périat, **V. Desfontaine**, S. Moco, D. Barron, J. Veuthey, D. Guillarme

11:20 ANYL **323.** Comprehensive subcritical fluid chromatography for the modern drug discovery lab. **T. Leek**, P. Sjo

Section C

Hilton San Francisco Union Square
Union Square 17/18

Chemical Forensics

Chemometrics & Statistics for Signature Discovery & Exploitation

Cosponsored by CHAL and PRES

J. R. Cort, R. Foster, J. J. Moran, *Organizers*

C. Fraga, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ANYL **324.** Statistical framework for establishing defensibility of chemical threat detection and forensics methods. **K. Jarman**, J.H. Wahl, K.L. Wahl

8:35 ANYL **325.** Wow! or the so-what? factor: A measured approach to the application of chemometrics to examine complex analytical data in forensic science. **C. McKenzie**, N. Nic Daéid

9:00 ANYL **326.** Establishing evidentiary value through validated inference and reporting of likelihood ratios. **M.E. Sigman**

9:25 ANYL **327.** Forensic analysis of diesel using GC×GC–TOFMS with Fisher Ratio Software. B.A. Parsons, D.K. Pinkerton, B.C. Reaser, **R.E. Synovec**, B. Wright

9:50 Intermission.

10:10 ANYL **328.** Assessment of one-class supervised pattern recognition methods for nuclear material group inclusion/exclusion. **C. Stork**

10:30 ANYL **329.** Rodenticide attribution signatures. **E. Durnal**, K. Brady, E.P. Naveo, N. Doll, C. Carroll, O. Beverly

10:50 ANYL **330.** DHS Chemical Forensics Program – REACTS. **K. Brady**, E. Durnal, P.J. Deardorff, K. Broekhuizen, C. Grisham

11:10 ANYL **331.** Comprehensive analysis of aquatic toxins by HPLC-MS/MS. B. Valenzuela, B. Kaiser, J. Arce, **D. Wunschel**

11:30 ANYL **332.** Infrared microscopy and multivariate curve resolution for the forensic examination of automotive paint chips and smears. **B.K. Lavine**, M. Allen, N.T. Perera, C.G. White, K. Kalkan, K. Nishikida

Section D

Hilton San Francisco Union Square
Franciscan C

Advanced Materials, Discovery, Characterization & Safety

L. A. Holland, *Organizer*

W. Zhong, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **333.** Metal nanoparticle fate and stability. **A.J. Haes**

9:00 ANYL **334.** Analytical assessment of protein conformational change induced by interaction with nanomaterials. **W. Zhong**, Y. Duan

9:55 Intermission.

10:10 ANYL **335.** Biomolecular screening of nanomaterials. **L.A. Holland**, T.A. Davis, M. Ellington

11:05 ANYL **336.** Growth-based Bacterial Viability (GBV) assay for interference-free and high-throughput nanotoxicity screening. **T.A. Qiu**, T. Nguyen, H. Frew, N. Hudson-Smith, D. Forester, P. Clement, A. Vartanian, L.M. Jacob, M. Hang, C.J. Murphy, R.J. Hamers, V. Feng, C.L. Haynes

Section E

Hilton San Francisco Union Square
Union Square 19/20

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of David R. Walt

Cosponsored by BIOT

J. M. Desimone, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 ANYL **337.** Nanoparticle-mediated characterization of circulating tumor cell subpopulations. **S.O. Kelley**

9:10 ANYL **338.** Spherical nucleic acids: Making a case for next-generation nucleic acid therapeutics. **C.A. Mirkin**

9:40 Intermission.

9:55 ANYL **339.** Microfabricated systems to screen and separate cells and tissues based on complex phenotypes. **N.L. Allbritton**

10:25 ANYL **340.** Chemiresistive sensors: Functionalization and organization of carbon nanotubes. **T.M. Swager**

10:55 ANYL **341. Award Address** (Kathryn C. Hach Award for Entrepreneurial Success sponsored by the Kathryn C. Hach Award Fund). Microwell arrays as a platform for discovery and diagnostics. D.R. Walt

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Catalysis

Sponsored by ENFL, Cosponsored by ANYL

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

TUESDAY AFTERNOON

Section A

Hilton San Francisco Union Square
Union Square 14

Synthesis & Characterization of Materials for Energy Applications

Novel Architectures, Materials & Synthetic Routes/In Operando & Surface Sensitive Analysis

Cosponsored by CATL

J. Rodriguez Lopez, D. R. Rolison, *Organizers*

K. J. Stevenson, *Organizer, Presiding*

J. W. Long, *Presiding*

1:30 ANYL **342.** Designing transition metal oxides for energy storage at high charge/discharge rates. H. Kim, J. Cook, S.H. Tolbert, **B. Dunn**

2:00 ANYL **343.** Understanding pseudocapacitive charge storage from fundamental interfacial processes to 3D electrode design. **J.W. Long**, M.D. Donakowski, J.F. Parker, M.B. Sassin, J.M. Wallace, D.R. Rolison

2:30 ANYL **344.** Revealing Li intermetallic transformations using operando neutrons and NMR methods. **A. Co**

3:00 Intermission.

3:30 ANYL **345.** Advanced transmission electron microscopy for Li-ion battery cathodes. **A. Abakumov**

4:00 ANYL **346.** Watching reactions with operando X-ray tools. **K.W. Chapman**

4:30 ANYL **347.** Engineering non-precious metal oxides as cathode electrocatalysts for Li-O2 batteries. **E. Nikolla**

Section B

Hilton San Francisco Union Square

Franciscan D

New Applications of Supercritical Fluid Chromatography

L. Miller, *Organizer*

L. Taylor, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ANYL **348.** Process excellence in discovery scale pharmaceutical chiral purifications. **Y. Zhang**, M. Beres, J. Carlson, G. Bi, S. Hollis, P. Krolikowski, L. Miller

1:35 ANYL **349.** Online Supercritical Fluid Extraction/Supercritical Fluid Chromatography (SFE/SFC) for pharmaceutical and food sample analysis. **M. Wong**, Y. Ko, A. Guillen, J.P. Pease

2:00 ANYL **350.** Stereo isomeric analysis of cannabinoids using UPC2. **J.L. Runco**, A. Aubin

2:25 ANYL **351.** Purification of cannabinoids using preparative SFC. **B. Murphy**

2:50 Intermission.

3:10 ANYL **352.** Advances and applications of supercritical fluid chromatography for small molecules medicinal chemistry. **G. Rosse**

3:35 ANYL **353.** Practical separation of synthetic peptides from complex crude mixtures by SFC. **M. Ventura**

4:00 ANYL **354.** New SFC developments as the extended tools for pharmaceutical analysis. **L. Zeng**

4:25 ANYL **355.** Applications of supercritical fluid technologies for the analysis, extraction and isolation of cannabinoids for cannabis-based therapeutics. **C.J. Hudalla**

4:50 Concluding Remarks.

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Section C

Hilton San Francisco Union Square

Union Square 17/18

Chemical Forensics

Isotopic & Elemental Profiling for the Source Attribution of Materials

Cosponsored by CHAL and PRES

J. R. Cort, R. Foster, C. Fraga, *Organizers*

J. J. Moran, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ANYL **356.** Forensic attribution using stable isotopes: Hairs to humans and insects to carrion. **G.P. Jackson**, R. Mohr, M.P. Matos, M. Engel

1:35 ANYL **357.** Applying isotope ratio mass spectrometry to characterize chemical threat agents: Case study on plastic explosives. **L. Chesson**, J. Howa, M. Lott, J. Ehleringer

2:00 ANYL **358.** Isotope composition of manufactured bulk ammonium nitrate and its isolated ions as a method of differentiating forensic samples. **B.L. Grimm**, L.A. Stern, A.J. Lowe, J. Buscaglia, J. Hietpas, C.M. Marsh

2:25 ANYL **359.** Linking a fentanyl sample to its synthetic origin using stable isotope forensic signature analysis. **M. Singleton**, C.A. Valdez, S. Hok, H.A. Mulcahy, B.P. Mayer, A.M. Williams

2:50 Intermission.

3:10 ANYL **360.** Signatures for detection and attribution of chemical agents and emerging threats using position specific isotope analysis (SNIF-NMR) and multimodal NMR at Ultra-Low Magnetic Field Strengths (ULMF). **R.F. Williams**, R. Michalczyk, M.A. Espy

3:35 ANYL **361.** Position-Specific stable isotope ratio measurement for chemical forensics. **J.R. Cort**, S.M. Colby, **R.S. Renslow**

4:00 ANYL **362.** Characterisation of international uranium ore concentrates and uranium ores for materials provenancing in nuclear forensics. **R. Popelka-Filcoff**, T. Ditcham, A. Wotherspoon, C. Lenehan, P. Kirkbride, A. Stopic, J. Bennett, T. Bull

4:25 ANYL **363.** Forensic applications of laser ablation ICP-MS. **J. Almirall**

Section D

Hilton San Francisco Union Square

Franciscan C

Advanced Materials, Discovery, Characterization & Safety

W. Zhong, *Organizer*

L. A. Holland, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ANYL **364.** Optical and electronic property of Au nanomaterials revisited. J. Zhang, J. Zhao, S. Sun, L. Swartz, S.L. Riechers, J. Zheng, **G. Liu**

2:00 ANYL **365.** Microbial community response to food and industrial grade titanium dioxide in decentralized wastewater treatment systems. T. Waller, **S.L. Walker**

2:55 Intermission.

3:10 ANYL **366.** Evaluation of electronic structure via voltammetry: A theoretical study of Carbon Nanotubes. **M. Hossain**, B. Muralidharan, B. Kirk

4:05 ANYL **367.** Spectroscopic single-molecule tracking reveals the one-dimensional diffusion pathways in surfactant-templated mesoporous silica. **R. Kumarasinghe**, **D.A. Higgins**, **T. Ito**

Section E

Hilton San Francisco Union Square

Union Square 19/20

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement: Symposium in Honor of Vicki H. Wysocki

Cosponsored by WCC

F. M. Fernandez, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ANYL **368. Award Address** (Frank H. Field & Joe L. Franklin Award for Outstanding Achievement in Mass Spectrometry sponsored by Waters Corporation). Development of surface-induced dissociation as a structural biology tool. V.H. Wysocki

1:55 ANYL **369.** Uncovering lipid connections – new roles for mass spectrometry. **C. Robinson**

2:15 ANYL **370.** Progress in top-down analysis of branched proteins. **C.C. Fenselau**, A. Lee, L. Geis-Asteggiante, S. Chauhan, D. Chen, Y. Wang, E. Dixon, D. Abeykoon, M. Miller, D. Fushman

2:35 ANYL **371.** Mapping peptide/protein conformation space: A challenge for IM-MS. **D.H. Russell**

2:55 Intermission.

3:10 ANYL **372.** Ultraviolet photodissociation mass spectrometry for characterization of protein complexes. **J. Brodbelt**

3:30 ANYL **373.** Accelerated reactions in microdroplets: Mechanisms and scale-up methods. **R.G. Cooks**

3:50 ANYL **374.** Distonic polyradical cations. **H.I. Kenttamaa**

4:10 ANYL **375.** Proto-Peptidomics: The first peptides in Darwin's warm little pond. J.G. Forsythe, A. Petrov, W.C. Millar, S. Yu, I. Mamajanov, R. Krishnamurthy, M. Grover, N.V. Hud, **F.M. Fernandez**

4:30 Concluding Remarks.

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Energy Sources & Combustion

Sponsored by ENFL, Cosponsored by ANYL

WEDNESDAY MORNING

Section A

Hilton San Francisco Union Square

Union Square 14

Synthesis & Characterization of Materials for Energy Applications

Fundamental & Molecular Models for Advanced Energy Materials/Novel Architectures, Materials & Synthetic Routes

Cosponsored by CATL

D. R. Rolison, K. J. Stevenson, *Organizers*

J. Rodriguez Lopez, *Organizer, Presiding*

H. White, *Presiding*

8:30 ANYL **376.** Electrochemistry at three-phase boundaries. **H. White**, S. German, Y. Liu, M. Edwards, Q. Liu, L. Luo, H. Ren

9:00 ANYL **377.** Interface characterization of PEDOT:PSS on solution-processed ITO using photoelectron spectroscopy. **L.M. Kogler**, M. Haeming, C. Heske

9:30 Intermission.

10:00 ANYL **378.** Ion transport in single-ion conducting polymer electrolytes for lithium batteries. **J.L. Schaefer**

10:30 ANYL **379.** Significance of manganese in designing advanced Li-ion battery cathodes. **M. Thackeray**

11:00 ANYL **380.** Controlling the arrangement of matter at different length scale in hybrid membrane to tune the ion transport. **C. Laberty**

Section B

Hilton San Francisco Union Square

Franciscan D

Active Learning in the Undergraduate Analytical Chemistry Curriculum

Cosponsored by CHED

T. J. Wenzel, *Organizer*

J. K. Robinson, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ANYL **381.** Overcoming obstacles to active learning in analytical chemistry. **J.K. Robinson**

8:55 ANYL **382.** Applying active learning to give students enduring learning experiences in chemistry at Texas A & M International University. **A.K. Addo-Mensah**

9:15 ANYL **383.** Active learning analytical chemistry laboratory; environmental applications and course embedded research performed on an island. **D.J. Lecaptain**, J. Tomasik

9:35 ANYL **384.** Particulate matter in public spaces: An exploratory, student-led air quality monitoring project for the third-year classroom. **S.A. Styler**, S. Gao

9:55 Intermission.

10:10 ANYL **385.** Quantitative determination of aluminum in eight deodorant brands. **A. Kanu**, V.M. Sedwick, A. Leal, D. Turner

10:30 ANYL **386.** Lithia Water Springs Project: Structuring active learning around a community resource. **S.C. Petrovic**

10:50 ANYL **387.** Football, Beer, and Analytical Chemistry: The Path to Significant Learning. **M.F. Tuchler**

11:10 ANYL **388.** Instrument building in undergraduate instrumental analysis. **L.A. Baker**

‡ *Cooperative Cosponsorship*

Section C

Hilton San Francisco Union Square
Union Square 17/18

Recent Innovations in Nano-Biosensing

X. Li, Y. Zeng, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ANYL **389.** Dynamic cantilever biosensors for pathogens, toxins and genes and NSF's nanobiosensing program. **R. Mutharasan**

9:05 ANYL **390.** Nanoporous gold: A multifunctional material for electrochemical detection and purification of nucleic acids in complex biological fluids. **E. Seker**

9:35 ANYL **391.** Nanoparticle-mediated photothermal immunosensing for quantitative biomarker detection using a thermometer. **X. Li**

10:05 Intermission.

10:20 ANYL **392.** Graphene FRET aptasensor built on a solid support. **Y. Ueno**, T. Teshima, C. Henderson, H. Nakashima

10:50 ANYL **393.** Amphiphilic nanoparticles as droplet stabilizers for high-fidelity droplet-based biochemical assays. **M. Pan**, S. Tang

11:20 ANYL **394.** Nanomaterial-Inspired microfluidic technologies for biomarker analysis. **Y. Zeng**

11:50 Concluding Remarks.

Section D

Hilton San Francisco Union Square
Franciscan C

Hierarchical Characterization of Materials Using Atomic Spectrometry & Related Techniques

U. E. Fittschen, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ANYL **395.** Mapping trace metals in hierarchical systems using X-ray fluorescence microscopy. **S. Vogt**

8:35 ANYL **396.** High-Resolution elemental imaging with LA-ICP-TOFMS: State of the art. **A. Gundlach-Graham**, G. Schwarz, M. Burger, P.S. Garofalo, B. Hattendorf, D. Günther

9:05 ANYL **397.** Solid sample analysis by a Tandem LIBS and LA-ICP-MS system. **J.J. Gonzalez**

9:35 Intermission.

9:45 ANYL **398.** X-ray tomographic imaging of mechanical deformation at various length and time scales. **B. Patterson**, J. Mertens, K. Henderson, N. Cordes, M. Herman, P.M. Welch, C.F. Welch, J. Williams, A. Sundar, N. Chawla, X. Xiao

10:15 ANYL **399.** Applications of x-ray tomography across multiple length scales. **P. Pianetta**

10:45 ANYL **400.** Practical multi-scale characterization with correlative microscopy. **J. Gelb**, L. Lavery, W. Harris, H. Bale, A. Merkle

11:05 ANYL **401.** Detecting the chemical phases of lithium and iron phosphate in nanoparticles with photoinduced force microscopy. **D. Nowak**, W. Morrison, R. Murdick, S. Park, J. Cabana

11:25 ANYL **402.** X-ray fluorescence *in-vivo* elemental imaging of plant samples. **U.E. Fittschen**, H. Kunz, R. Hoehner, I.M. Tyssebotn, A. Fittschen

11:45 Concluding Remarks.

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Fuel Cells

Sponsored by ENFL, Cosponsored by ANYL

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

WEDNESDAY AFTERNOON

Section A

Hilton San Francisco Union Square
Union Square 14

Synthesis & Characterization of Materials for Energy Applications

Novel Architectures, Materials & Synthetic Routes

Cosponsored by CATL

D. R. Rolison, *Organizer*

J. Rodriguez Lopez, K. J. Stevenson, *Organizers*, *Presiding*

1:30 ANYL **403.** In-depth study of non-intercalation materials as electrode materials for high energy Na-ion batteries and Li-ion batteries. **S. Meng**

2:00 ANYL **404.** Alkali and transition metal fluoride-phosphates as cathode materials for metal-ion batteries. **E. Antipov**

2:30 ANYL **405.** Design of stable polymer- and ionic liquid-based electrolytes for Li-O2 batteries. **S. Feng**, L. Giordano, C. Amanchukwu, M. Chen, R. Anandakathir, J.A. Johnson, Y. Shao-Horn

3:00 Intermission.

3:30 ANYL **406.** Effects of nanoscale interfacial design on the UV and visible photocatalytic activity of plasmonic aerogels. **J.J. Pietron**, P.A. DeSario, T.H. Brintlinger, R.M. Stroud, D.R. Rolison

4:00 ANYL **407.** Characterization of composite materials prepared by controlled reassembly of functional nanosheets. Q. Cheng, **C.K. Chan**

4:30 ANYL **408.** Synthesis of crystalline metal chalcogenide electrocatalysts and group III-V semiconductor films from aqueous solutions at room temperature. **S. Maldonado**

Section B

Hilton San Francisco Union Square
Franciscan D

Active Learning in the Undergraduate Analytical Chemistry Curriculum

Cosponsored by CHED

T. J. Wenzel, *Organizer*

J. K. Robinson, *Organizer, Presiding*

1:30 ANYL **409.** Optical properties of gold nanoparticles: A contextual module to introduce concepts of chemical equilibrium and spectrophotometry. **A.G. Cavinato**

1:50 ANYL **410.** Optimization of an HPLC method: A method development approach to upper-level undergraduate laboratory instruction. **T. Thomas-Smith**

2:10 ANYL **411.** 3D Printing, active learning, and undergraduate instrumental analysis. **B.J. Winters**

2:30 ANYL **412.** How do you sample all of the leaves in the forest? . **M. Kistler Langston**

2:50 Intermission.

3:05 ANYL **413.** Empowering active learning with virtual machines. K. Streu, N.C. Lee, A. Zubiria, S. Anderson, S. Gagliardi, **R.M. Georgiadis**

3:25 ANYL **414.** Electrode modification through self-assembly and electron transfer characterizations by cyclic voltammetry and electrochemical impedance spectroscopy. **J. Yan**

3:45 ANYL **415.** Articles from the primary literature as a platform for active learning. **M.L. Kovarik**

4:05 Concluding Remarks.

Section C

Hilton San Francisco Union Square
Union Square 17/18

Recent Innovations in Nano-Biosensing

X. Li, *Organizer*

Y. Zeng, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ANYL **416.** Molecularly imprinted nanoparticles as non-animal antibodies substitutes for detection of viruses. **A. Poma**, K. Karim, G. Battaglia, S. Piletsky

1:55 ANYL **417.** Nanopatterned matrices enable enzyme activity measurements using SAMDI-mass spectrometry. **M. Cabezas**, C.A. Mirkin, M. Mrksich

2:15 ANYL **418.** Development of DNA-based glycan microarray platform for on-chip enzymatic glycosylation. **H. Heo**, C. Kim, J. Seo, H.J. Cha

2:35 ANYL **419.** Development of genetically engineered virus for bacteria detection in resource-limited settings. **J. Chen**, S. Nugen

2:55 ANYL **420.** Development and characterization of thiol-responsive scintillation proximity assay core-shell nanoparticles as turn-on biosensors. **Z. Mokhtari**, C. Janczak, C.A. Aspinwall

3:15 Intermission.

3:25 ANYL **421.** Janus micromotors for electrochemical sensing and biosensing. **B. Jurado**, M. Pacheco, J. Rojo, A. Escarpa

3:45 ANYL **422.** Charge-directed immobilization of bacteriophage on nanostructured electrode for whole cell electrochemical biosensors. **Y. Zhou**, R. Ramasamy

4:05 ANYL **423.** Membrane protein ion channels as specific molecule sensors. **R. Lazenby**, F. Macazo, R.J. White

4:25 Concluding Remarks.

Section D

Hilton San Francisco Union Square
Franciscan C

Applications of Wearable or Implantable Sensors for Systems in Biology

L. Deravi, T. Zarkovic Grove, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ANYL **424.** 3D Printing functional electronic and bioelectronic devices. **M.C. McAlpine**

1:35 ANYL **425.** Electroactive protein-based materials. **L.F. Deravi**

2:05 Intermission.

2:20 ANYL **426.** Towards the development of wearable biosensors for human performance. **R.R. Naik**

2:50 ANYL **427.** Chemical sensors: Flexibility and economy by putting technology into transducing materials. **T.M. Swager**

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Gas Storage & Ion Conduction

Sponsored by ENFL, Cosponsored by ANYL

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Frontiers in Glycoanalytics

MS & NMR Methods

Sponsored by CELL, Cosponsored by ANYL, CARB‡ and MPPG‡

WEDNESDAY EVENING

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Sponsored by ENVR, Cosponsored by ANYL

Contaminants of Emerging Concern in Natural & Engineered Systems

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Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences

Sponsored by ENVR, Cosponsored by ANYL and CHED

THURSDAY MORNING

Section A

Hilton San Francisco Union Square
Union Square 14

Advances in Analytical Electrochemistry

L. A. Baker, *Organizer, Presiding*

8:30 ANYL **428.** Synthesis and characterization of highly active Au NPs using the rotating disk slurry electrodepoition technique for EtOH electrooxidation in alkaline media. **L. Betancourt**

8:50 ANYL **429.** Perfluoroalkyl and alkyl modified glassy carbon electrodes: A model system to understand role of solvation in interfacial electron transfer kinetics. **S. Mao**, H. Sun

9:10 ANYL **430.** Use of nonstandard pH electrodes for the determination of pH-values of e-cigarette aerosols to comply with requiremnts specified in USFDA draft guidance on Premarket Tobacco Product Applications (PMTA) for Electronic Nicotine Delivery Systems (ENDS). **J.H. Lauterbach**

9:30 ANYL **431.** Use of electrochemical techniques in conjunction with computer simulations and spectroscopic methods to determine the electrochemical reduction pathways of atrazine. **J. Brown**

9:50 ANYL **432.** Using voltammetry to detect hydrogen-bonding interactions. **R.D. Webster**

10:10 Intermission.

10:30 ANYL **433.** SECM with high areal scan rates using continuous line probes and compressed sensing. G. O'Neil, H. Kuo, J. Wright, **D. Esposito**

10:50 ANYL **434.** PeakForce scanning electrochemical microscopy with nanoelectrode probes. **Z. Huang**, R. Poddar, P. De Wolf

11:10 ANYL **435.** Localized detection of D-serine using scanning electrochemical microscopy and an enzymatic biosensor. **D. Polcari**, S.C. Perry, L. Pollegioni, M. Geissler, J. Mauzeroll

11:30 ANYL **436.** Electrochemical gate-controlled conductance switching in DNA via STM break junction technique. **L. Xiang**, J.L. Palma, Y. Li, V. Mujica, M.A. Ratner, N. Tao

Section B

Hilton San Francisco Union Square

Franciscan D

Advances in Analytical Mass Spectrometry

K. Phinney, *Organizer, Presiding*

8:30 ANYL **437.** Role of acetylation in validating the peptide sequence using mass spectrometry: Implications in proteomics. **M. Jagannadham**

8:55 ANYL **438.** Using mass spectrometry and small molecule reagents to detect distinctive structural features of different prion conformations (strains). **C.J. Silva**, M.L. Erickson-Beltran, I.C. Dynin

9:20 ANYL **439.** Withdrawn.

9:45 ANYL **440.** Laser desorption/ionization droplet delivery mass spectrometry for live single cell analysis and imaging. **J. Lee**, H. Nam, R.N. Zare

10:10 Intermission.

10:25 ANYL **441.** Sub-Minute comprehensive metabolomic analyses of biofluid and environmental samples using SPE-IMS-MS. **E.S. Baker**, X. Zheng, N. Aly, V. Paurus, R.F. Marek, K.C. Hornbuckle, R.S. Renslow, D. Thomas, J. Teeguarden, T. Metz, R. Smith

10:50 ANYL **442.** Application of statistical sample classification in non-target analysis of complex environmental samples analyzed via LC-HR-QTOFMS. **S. Samanipour**, J.A. Baz-Lomba, M.J. Reid, B. Van Bavel, K. Thomas

11:15 ANYL **443.** Taking on mass spectrometry challenges with MethodsNow™. **J.M. Wilson**, S.P. Kuhn

Section C

Hilton San Francisco Union Square

Union Square 17/18

Advances in Analytical Spectroscopy

J. M. Harris, *Organizer*

J. C. Lee, *Presiding*

8:00 ANYL **444.** DNA micelle flares: A study of the basic properties that contribute to enhanced stability and binding affinity in complex biological systems. **Y. Wang**, W. Tan

8:25 ANYL **445.** Ultra-highly sensitive and dynamic fluorescence imaging of ROS in live cells and in vivo. **P. Li**

8:50 ANYL **446.** Advancing spectroscopy of buried interfaces: Determination of surface potential and electrical double-layer structure at the aqueous electrolyte-nanoparticle interface. **M.A. Brown**

9:15 ANYL **447.** Fluorinated boronic acid-appended pyridinium salts for Diol recognition & discrimination in water using 19F NMR. **J. Axthelm**, A. Schiller

9:40 Intermission.

10:00 ANYL **448.** Speciation of trace amounts of organic carbon with NMR: The example of plant silica particles. **A. Masion**, A. Alexandre, F. Ziarelli, S. Viel, G. Santos

10:25 ANYL **449.** Quantitative analysis of organically bound minerals in nutritional supplements using FT-IR spectroscopy. **C. Connolly**, R. Murphy

10:50 ANYL **450.** FTIR microspectroscopy imaging reveals changes in adipose tissues and liver induced by high-fat diet. **S.P. Liyanage**, A. Bouyanfif, N. Abidi, L. Ramalingam, N. Moustaid-moussa

11:15 ANYL **451.** Microfluidics-Based surface plasmon resonance for biomolecular interactions and detection of biomarkers related to neurological disorders. **X. Wang**, E. Enriquez, N. Ukhlivanova, A. Benedict, Y. Wang, F. Zhou

Section D

Hilton San Francisco Union Square

Franciscan C

Applications of Wearable or Implantable Sensors for Systems in Biology

L. Deravi, T. Zarkovic Grove, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ANYL **452.** Wearable epidermal microfluidic systems capable of capture, storage and colorimetric sensing of sweat. **A. Koh**, D. Kang, J.A. Rogers

8:50 ANYL **453.** Implantable indium gallium zinc oxide field effect biosensors. X. Du, **G.S. Herman**

9:20 ANYL **454.** Mechanically adaptive bio-nanocomposites for implantable sensing. **J. Foster**

9:50 ANYL **455.** Nanocellulose wearable sensor platform. Y.S. Kim, **S. Minko**

10:20 Intermission.

10:35 ANYL **456.** Low-Cost human and animal health diagnostics enabled through novel hybrid microfluidic systems. K. Ramzy, C. Heist, G. Bandara, S. Pengpumkiat, **V.T. Remcho**

11:05 ANYL **457.** Microbial sensing – learning from the innate immunity receptors. **T. Zarkovic Grove**, R. Parker, A. Mercedes-Camacho

11:35 ANYL **458.** Towards the development of a smart device surface to non-ivasively image and monitor implant associated infection in-situ. **U. Uzair**, J.N. Anker

11:50 Concluding Remarks.

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Frontiers in Glycoanalytics

Molar Mass & Crystallinity Analyses

Sponsored by CELL, Cosponsored by ANYL, CARB‡ and MPPG‡

THURSDAY AFTERNOON

Section A

Hilton San Francisco Union Square

Union Square 14

Advances in Analytical Electrochemistry

L. A. Baker, *Organizer, Presiding*

1:00 ANYL **459.** Highly sensitive and selective electrochemical biosensor for monitoring sialic acid in live brain of mice with Alzheimer's disease based on wettability switching of a stimuli-responsive copolymer. **S. Ding**, C. Ma, A. Zhu, G. Shi

1:20 ANYL **460.** Biosensors based on conducting polymer scaffolds targeting carbohydrate-protein interactions. **A. Rehman**, **M. Sharif**

1:40 ANYL **461.** Lab-on-paper cyto-device for the detection of H2S released from MCF-7 cells. **J. Yu**, **L. Zhang**, **Y. Zhang**, **S. Ge**, **M. Yan**, **H. Liu**

2:00 ANYL **462.** Highly selective nanoparticle-enhanced electrochemical biosensing platforms for proteins in biological fluids. **H. Lee**, Y. Si, S. Hayati

2:20 Intermission.

2:40 ANYL **463.** DNA biosensing through instantaneously electrostatic attraction on polystyrene gold electrode. **B. Yao**, W. Lu, Q. Yuan

3:00 ANYL **464.** Integration of collagen hydrogel scaffold to enhance performance of RNA Electrochemical-Aptamer Based (E-AB) sensors. **M. Santos Cancel**

3:20 ANYL **465.** Real-time monitoring of Ca2+ and pH using a non-invasive wearable biosensor. **H.Y. Nyein**, W. Gao, A. Javey

3:40 ANYL **466.** Real-time parallel detection of alpha-L-fucosidase and cardiac troponin I with an ultrasensitive plasmonic biosensor. **X. Han**, H. Shokri Kojori, S. Kim, R.M. Leblanc

Section B

Hilton San Francisco Union Square

Franciscan D

Advances in Analytical Mass Spectrometry

K. Phinney, *Organizer, Presiding*

1:00 ANYL **467.** Trace determination of nitrosamines in finished drinking water by direct-inject LC-MS/MS. **A.E. Pierri**

1:25 ANYL **468.** 2-Hydrazinyl-N, N, N-trimethylethan-1-ammonium iodide: A reagent for chemoselective isolation of volatile aldehydes and ketones from exhaled breath. **M. Ogunwale**, X. Fu, M.H. Nantz

1:50 ANYL **469.** High-throughput gas and headspace analysis for the process-line and laboratory: SIFT-MS. V.S. Langford, **B.J. Prince**, D.B. Milligan, M. Perkins, T. Wilks, T. Potter

2:15 ANYL **470.** Identifying known unknowns: A comparison between ChemSpider and the US EPA's CompTox Dashboard. **A. McEachran**, J. Sobus, A.J. Williams

2:40 Intermission.

2:55 ANYL **471.** Novel method for determining aldehyde and ketone photoproducts from solar irradiated crude oil-seawater systems by MS/MS. X. Cao, **M.A. Tarr**

3:20 ANYL **472.** Positive mode atmospheric pressure chemical ionisation mass spectrometry in archaeological analyis: Differentiation of epimers of pentacyclic terpenoids. **W. Martin**, R.D. Bowen, R. Brettell, R. Gallagher, C. Townley

3:45 ANYL **473.** Personal information from latent fingerprints obtained by mass spectrometry using machine learning. **Z. Zhou**, R.N. Zare

Section C

Hilton San Francisco Union Square

Union Square 17/18

Advances in Analytical Spectroscopy

J. M. Harris, *Organizer*

S. R. Emory, *Presiding*

1:00 ANYL **474.** Conformation and dynamics of -synuclein probed by Raman microspectroscopy. J.D. Flynn, **J.C. Lee**

1:25 ANYL **475.** Harnessing drop coat deposition Raman spectroscopy for non-invasive cancer diagnosis. **A. Niyibizi**, J. Jabara, R. Halvorson, S. Potter, C. Lahr, C. Gomez, M. Sakiyama

1:50 ANYL **476.** *In situ* determination of metformin in Type 2 diabetes tablets using Raman spectroscopy. **S.A. Oladepo**

2:15 ANYL **477.** Towards a nonresonant detection strategy for single molecule SERS. **N.L. Wong**, R.P. Van Duyne

2:40 Intermission.

3:00 ANYL **478.** Nanostructured thin-film materials for surface-enhanced Raman scattering and electrochemical studies. **S.R. Emory**, C. Swanson, E. Douglass

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

3:25 ANYL **479.** Breakthrough developments in x-ray spectroscopy toward LA-ICP-MS capabilities: Trace-Level microns-scale mapping and femtogram detection sensitivity. **S. Lewis**, W. Yun, S. Lau, B. Stripe, D. Reynolds, A. Lyon, J. Kirz, S. Chen, V. Semenov, M. Cordier

3:50 ANYL **480.** Recent advances in two-dimensional X-ray diffraction. **B.B. He**

Section D

Hilton San Francisco Union Square
Franciscan C

Applications of Wearable or Implantable Sensors for Systems in Biology

L. Deravi, T. Zarkovic Grove, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ANYL **481.** Comprehensive investigation of potential adverse effects of silver nanoparticle and its environmental transformation in embryonic zebrafish using implantable biosensor. **X. Liu**, E. Dumitrescu, K. Wallace, S. Andreescu

1:20 ANYL **482.** Nanosensor for chemical imaging of neurotransmitter acetylcholine using MRI. **Y. Luo**, E.H. Kim, H. Clark

1:35 ANYL **483.** Silk: A glamorous bridge between fashion and smart outfits. **G. Matzeu**, P. Tseng, L. Mogas-Soldevila, B. Napier, L. Garbarini, D.L. Kaplan, F. Omenetto

2:05 ANYL **484.** Peptide melanins. **R. Ulijn**

2:35 Intermission.

2:50 ANYL **485.** Wearable sweat biosensors for personalized healthcare. **W. Gao**, H. Nyein, Z. Shahpar, A. Javey

3:05 ANYL **486.** Biomaterials-based energy storage devices for next generation edible electronics. **Y. Kim**

3:35 ANYL **487.** Metal organic frameworks for portable chemical sensing. **K. Mirica**, M.K. Smith, M. Ko, A. Aykanat

4:05 Concluding Remarks.

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

BIOT

Division of Biochemical Technology

M. O'Malley and V. Roy, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Cellulose Structure & Biosynthesis (see *CELL, Sun, Mon, Tue*)

Innovations in Drug Delivery Systems & Combination Products (see *PMSE, Tue, Wed*)

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of David R. Walt (see *ANYL, Tue*)

Science for a Sustainable Energy Future (see *PRES, Mon*)

Young Investigator's Symposium (see *PMSE, Sun, Mon*)

Undergraduate Research Posters (see *CHED, Mon*)

SOCIAL EVENTS:

Membership Desk, 8:00 AM: Sun, Mon, Tues, Wed, Thu

Reception, 6:30 PM: Sun

Program Chair's Lunch, 12:30 PM: Wed

Company Seminars, 12:30 PM: Sun, Mon, Tue, Wed

Networking/Mentoring Session, 6:00 PM: Wed

BUSINESS MEETINGS:

BIOT Executive Committee Meeting, 7:00 PM: Mon

Future Programming Meeting, 12:30 PM: Tues

SUNDAY MORNING

Section A

InterContinental San Francisco
Grand Ballroom A

Upstream Processes

Disruptive Bioprocessing & Process Integration

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

N. R. Boyle, A. Ouyang, *Presiding*

8:30 BIOT **1.** Online capacitance probes precisely control cell biomass growth through temperature regulation. **J.C. Swanberg**, R. Lewis, K. Aron, M.C. Borys, Z. Li

8:50 BIOT **2.** Effective and efficient approaches to cell line engineering in CHO cells. **S. Sandefur**, C. Frye

9:10 BIOT **3.** Feasibility study of dielectric spectroscopy as a tool for monitoring and controlling of mammalian cell culture processes. **A. Zhang**, F. Ma, S. Ghose, O.D. Velev

9:30 BIOT **4.** Leveraging media components to control cell growth and improve specific productivity in perfusion cell culture. **S. Wang**, A. Lee-Goldman, J. Goby, J. Ravikrishnan, L. Zheng, S. Mishra, J.L. Coffman, H. Lin

9:50 Intermission.

10:10 BIOT **5.** Non-mammalian expression systems for new bioprocesses: Enabling a step-change in manufacturing productivity and cost. **M. Bartlett**, C. Wright, A. Kuo, N. Colant, M. Westoby, J.C. Love

10:30 BIOT **6.** Molecular mechanisms of epigenetic instability control in long-term cell culture processes. **M. Kamga**, S. Yoon

10:50 BIOT **7.** Integrated bioprocess for production of recombinant butyrylcholinesterase from transgenic rice cell suspension cultures. **J. Corbin**, S. Alkanaimsh, M. Kailemia, K. Karuppanan, R. Rodriguez, C.B. Lebrilla, K. McDonald, S. Nandi

11:10 BIOT **8.** Establishing a high-efficient serum-free process for influenza vaccine production using MDCK cells. **Q. Ye**, X. Liu, W. Dai, L. Zhao, Y. Wu, W. Peng, K. Hu, W. Tan

Section B

InterContinental San Francisco
InterContinental C

Downstream Processes

Advances in Chromatographic Separations

R. Barros, V. Natarajan, N. Tugcu, *Organizers*

D. J. Roush, *Organizer, Presiding*

J. Neville, A. Podgornik, *Presiding*

8:30 BIOT **9.** Aggregation phenomena in cation exchange chromatography and implications to process development for mAb and Fc-fusion proteins. **Z. Chen**, C. Huang, N. Chennamsetty, X. Xu, Z. Li

8:50 BIOT **10.** Competitive binding kinetics of antibody monomer-dimer mixtures on CEX resins during separation by frontal analysis. **J.M. Reck**, T.M. Pabst, A.K. Hunter, G. Carta

9:10 BIOT **11.** Understanding the molecular details of protein adsorption in polymer-grafted ion exchangers. J. Basconi, G. Carta, **M.R. Shirts**

9:30 BIOT **12.** Investigating domain contributions to antibody retention in chromatography systems. **J. Robinson**, D.J. Roush, S.M. Cramer

9:50 Intermission.

10:10 BIOT **13.** *In silico* scale-up from laboratory to production scale: A case study on applying mechanistic modeling for describing chromatographic purification of a monoclonal antibody. **F. Stueckler**, T. Hartneck, S. Paschen, K. Doninger, J. Griesbach

10:30 BIOT **14.** Enablers for QbD implementation: Mechanistic modeling for ion-exchange membrane chromatography. **L. Kanwar**, A.S. Rathore, A.P. Manvar

10:50 BIOT **15.** From bed to bead and below: Multiscale measurements of chromatography. **D.G. Bracewell**

11:10 BIOT **16.** Modeling of axial and radial heterogeneity of preparative chromatography packings. **M. Dorn**, D. Hekmat, D. Weuster-Botz

Section C

InterContinental San Francisco
Union Square

Biophysical & Biomolecular Processes

Protein Developability: Assessing Candidates for Preclinical & Clinical Studies

J. Moore, J. A. Van Deventer, *Organizers*

B. E. Jones, P. M. Tessier, *Presiding*

8:30 BIOT **17.** Measuring physical stability using intrinsic fluorescence and static light scattering. **K. Tschudi**, Y. Adem

8:50 BIOT **18.** Chemical unfolding as a predictor for monoclonal antibody stability. **J. Floyd**, A. Gillespie, C. Siska, B. Kerwin

9:10 BIOT **19.** Assessing differential photosensitivity of tryptophan using a model Trp-cage peptide as a mAbs surrogate. **L.F. Welch**, M. Deshpande, G. Deperalta, S. Alavattam, J. Lin

9:30 BIOT **20.** Non-ideal colligative properties in high concentration mAb solutions and impact to biopharmaceutical manufacturing. **A. Teran**, B. Callahan, R. Kaushik

9:50 Intermission.

10:10 BIOT **21.** Is the dilute solution diffusion interaction parameter a robust predictor of concentrated monoclonal antibody formulation shear viscosity? **J.A. Pathak**, S. Banappagari, A.L. Chamberlain, L. Lofchy, L. Kueltzo

10:30 BIOT **22.** Small volume screening of bispecific antibody solution viscosities. **M. Woldeyes**, L. Josephson, D. Leiske, W.J. Galush, E.M. Furst

10:50 BIOT **23.** Protein interactions at concentrated conditions and their impact on the thermodynamics and rheology of antibody solutions. **M.A. Blanco**, H.W. Hatch, J.E. Curtis, V.K. Shen

11:10 BIOT **24.** Multidimensional data visualization and data mining for characterization of long term protein phase behavior. **M. Klijn**

Section D

InterContinental San Francisco
Telegraph Hill

Bio-Based Products

Synthetic Biology Approaches to Engineer Production of Biofuels & Value-Added Chemicals

M. R. Antoniewicz, C. A. Eckert, G. Sriram, *Organizers*

A. Garst, Z. Shao, *Presiding*

8:30 BIOT **25.** Accelerating strain engineering with CRISPRi-based tool development. **B.F. Cress**, R.J. Linhardt, M. Koffas

8:50 BIOT **26.** Exploring nonconventional yeasts to produce pharmaceutical precursors and cosmetics additives. M. Cao, L. Zhao, **Z. Shao**

9:10 BIOT **27.** What does it take to engineer microbes for industrial applications? . **G. Stephanopoulos**

9:50 Intermission.

10:10 BIOT **28.** Production of branched-chain fatty acid and derivatives in high percentage. **W. Jiang**, G.J. Bentley, J.B. Qiao, F. Zhang

10:30 BIOT **29.** Inducible gene circuits to control *Saccharomyces cerevisiae* metabolism for advanced biofuel production. **E.M. Zhao**, J.L. Avalos

10:50 BIOT **30.** Robust and scalable two-stage fermentation for efficient terpenoids production using dynamic metabolic control. **Z. Ye**, M. Lynch

11:10 BIOT **31.** Engineering biosynthetic routes to high-performance non-natural polymers. **B. Motta Nascimento**, N.U. Nair

Section E

InterContinental San Francisco

Sutter

Biosimilars

Scientific Challenges in Production of Biosimilars: Processing & Analysis

R. S. Gronke, A. S. Rathore, *Organizers*

N. Chirmule, R. I. Shpritzer, *Presiding*

8:30 BIOT **32.** FDA perspective on demonstrating analytical similarity. **M.A. Shapiro**

9:10 BIOT **33.** Control of cell culture variables to meet target process and product quality in the production of biologics. **P. Bhebe**

9:30 BIOT **34.** Clearance of mAb charge variant by preparative ion exchange or multimodal chromatography. **T. Bjorkman**, **A. Ljunglöf**

9:50 Intermission.

10:10 BIOT **35.** Correlating critical quality attributes in IgG1: Glycosylation and charge heterogeneity. **N. Nupur**, R. Gudihal, A.S. Rathore

10:30 BIOT **36.** Addressing the challenge of higher-order structure assessment of biologics with 2D NMR. **J.P. Marino**

10:50 BIOT **37.** Withdrawn.

11:10 Panel Discussion.

Section F

InterContinental San Francisco

Grand Ballroom B/C

David Perlman Memorial Lectureship

M. A. O'Malley, T. M. Przybycien, V. Roy, *Organizers*, *Presiding*

11:30 BIOT **38.** Synthetic biology platforms for natural product biosynthesis and discovery. **C.D. Smolke**

Cellulose Structure & Biosynthesis

In the Plant Cell Wall

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

SUNDAY AFTERNOON

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Mammalian Cell Culture Process Development

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

M. Cunningham, N. George, S. W. Harcum, *Presiding*

2:00 BIOT **39.** Identification of genes that rescue deficient DNA double-strand break repair in Chinese hamster ovary cells. **X. Zhang**, K. Lee

2:20 BIOT **40.** Strategy to enhance monoclonal antibody productivity in CHO cells with anti-apoptotic inhibitors based on flow cytometric analysis. **D.W. Lin**, D. Townsend, A. Zanghi, P. Huang

2:40 BIOT **41.** Strategies to modulate CHO cell growth and reduce cell bleed product loss in high density perfusion cultures using classic cell culture medium nutrients. **D. Ogawa**, J. Ravikrishnan, S. Wang, H. Lin

3:00 BIOT **42.** Kinetic based metabolic model of mammalian cell cultures – model building and experimental validation for productivity improvement. **Z. Huang**, S. Yoon

3:20 Intermission.

3:40 BIOT **43.** Practical approach in bioreactor scale-up and process transfer. **S. Xu**, L. Hoshan, R. Jiang, B.M. Gupta, E. Brodean, J.S. Bowers, K. O'Neill, T. Seamans, H. Chen

4:00 BIOT **44.** Oxygen uptake modeling for cross-scale prediction of gas sparge rates in a CHO cell culture process. **B. Reed**, E. Garr

4:20 BIOT **45.** Elucidating the effects of CO2 on CHO cell metabolism in bioprocessing. **W. Chen**, J. Wang, **L. Zhao**, L. Fan, W. Tan

4:40 BIOT **46.** Novel shear assay for increasing chinese hamster ovary cell culture robustness in biomanufacturing. **D. Chang**, K. Chang, R. Ferguson, D. Osborne, O.D. Velev

Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Advances in Chromatographic Separations

R. Barros, V. Natarajan, N. Tugcu, *Organizers*

J. Neville, D. J. Roush, *Organizers*, *Presiding*

A. Podgornik, *Presiding*

2:00 BIOT **47.** Role of more than 40 years of improvement in protein A chromatography in the growth of the therapeutic antibody industry. **G. Bolton**, K. Mehta

2:40 BIOT **48.** Comprehensive evaluation of emerging anion exchange adsorber technologies for improving capacity and manufacturing agility. **M.R. McGarrah**, H. Ardeshna, G.J. Terfloth, K.E. Goklen

3:00 BIOT **49.** Evaluation of single-use FibroSelect technology for monoclonal antibody purification. **K. Mehta**, A. Venkatesh, I. Scanlon, P. Shah, R.G. Soderquist

3:20 Intermission.

3:40 BIOT **50.** Clearance of challenging, hard-to-remove CHO host-cell proteins by application of orthogonal approaches towards establishment of a robust downstream process. **N. Sanaie**, A. Velayo, A. Quezada, R. Vonder Reith, C. Tran, B. Kluck, J. Woo, C. Garcia, R. Krishnan

4:00 BIOT **51.** Chromatofocusing of IgG isoforms using peptide-based affinity adsorbents and dual ionic strength-pH gradients. **H. Reese**, J. Lembo, A. Hirsh, S. Menegatti

4:20 BIOT **52.** Developing a split-intein based platform for the purification of any biological therapeutic protein. **A. Lahiry**, J. Taris, M. Cooper, Y. Fan, T. Han, C. Shi, D.W. Wood

4:40 BIOT **53.** Rapid optimization of chromatographic separations using a nano-liter scale column in a microfluidic platform. **A. Azevedo**, I.F. Pinto, R.R. Soares, V. Chu, J.P. Conde, M.R. Aires-Barros

Section C

InterContinental San Francisco

Union Square

Biophysical & Biomolecular Processes

Protein Engineering & Design

J. Moore, J. A. Van Deventer, *Organizers*

A. J. Karlsson, J. Scheer, *Presiding*

2:00 BIOT **54.** Impact of affinity maturation on the specificity of antibodies targeting protein post-translational modification sites. D. Li, **Y. Cho**

2:20 BIOT **55.** Improved antibody library design and selection methods for minimizing trade-offs between affinity, specificity and stability. **K. Tiller**, M. Julian, L. Rabia, L. Li, S. Garde, S. Kumar, P.M. Tessier

2:40 BIOT **56.** Translatable affibody ligand discovery: Engineered biopanning, deep sequence-guided library design, and pharmacokinetic modulation. L. Stern, D. Woldring, B. Case, **B. Hackel**

3:00 BIOT **57.** Engineering the substrate specificity and activity of human proteases towards therapeutic target proteins: An approach to the treatment of autoimmune and inflammatory bowel diseases. **C.A. Denard**, L. Yi, J. DeSautelle, Z. Bennett, P. Marek, J. Taft, R. Yaghi, G. Georgiou, B. Iverson

3:20 Intermission.

3:40 BIOT **58.** Structurally guided design of chimeric proteins containing novel peptide loops. **J. Plaks**, J.R. Uzarski, T.J. Lawton, S. Filocamo, J. Kaar

4:00 BIOT **59.** Engineering histatin 5 for improved resistance to secreted aspartic proteases. S.P. Ikonomova, Y. Wang, **A.J. Karlsson**

4:20 BIOT **60.** Developing strategies to engineer G protein-coupled receptor binding properties. **J. Yoo**, P. Daugherty, M.A. O'Malley

4:40 BIOT **61.** Nicking mutagenesis: User-defined, single-pot comprehensive mutagenesis. **T. Whitehead**, E. Wrenbeck

Section D

InterContinental San Francisco

Telegraph Hill

Bio-Based Products

Synthetic Biology Approaches to Engineer Production of Biofuels & Value-Added Chemicals

M. R. Antoniewicz, C. A. Eckert, G. Sriram, *Organizers*

A. Garst, Z. Shao, *Presiding*

2:00 BIOT **62.** High-throughput enzyme screening platform for IPP-bypass MVA pathway for isopentenol production. **A. Kang**, C. Meadows, N. Canu, J.D. Keasling, **T. Lee**

2:20 BIOT **63.** New paradigm for pathway engineering at high-throughput and resolution. **M. Bassalo**, A. Garst, R.T. Gill

2:40 BIOT **64.** Industrialization of biology: Making nature accessible and affordable. **H. Tseng**

3:00 BIOT **65.** Multilevel engineering of the upstream aromatic module in *Saccharomyces cerevisiae* for high production of polymer and drug precursors. **M. Suastegui**, Z. Shao, C.Y. Ng, C. Maranas

3:20 Intermission.

3:40 BIOT **66.** Optimization of hexanoic acid production pathway in a recombinant *Escherichia coli* by precise flux rebalancing using synthetic promoters and UTRs. **S. Kim**, S. Jang, B. Sang, G. Jung

4:00 BIOT **67.** Dynamic metabolic control: Improved flux through malonyl-CoA for renewable production of valuable chemicals. **C. Cooper**, M. Lynch

4:20 BIOT **68.** Elucidating the influence of horizontal gene transfer and mutation rate on adaptive laboratory evolution for industrial biocatalyst development. **G.L. Peabody**, K.C. Kao

4:40 BIOT **69.** Whole genome regulator mutant library for expedited identification of beneficial mutations for enhanced tolerance towards environmental stress. **A. Choudhury**, Z. Wang, R.T. Gill, J. Kaar

Cellulose Structure & Biosynthesis

Evolution of Synthases & Fine Structure of Microfibrils

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

SUNDAY EVENING

Section A

InterContinental San Francisco

Grand Ballroom A

Startup Road

BIOT Tank

G. Bolton, A. May, T. Meyerrose, *Organizers*, *Presiding*

5:00 Panel Discussion.

MONDAY MORNING

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Mammalian Cell Culture Process Development

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

M. Cunningham, Y. Inn, *Presiding*

8:30 BIOT **70.** Ornithine concentration as a tool for modulating high mannose levels in mammalian cell culture. **H. Barkhordarian**, C. Huang, P.K. Chan, Z. Zhang, B. Shah, S. Kang, P.V. Bondarenko, C. Goudar

8:50 BIOT **71.** Impact of high osmolality cell culture media on cell growth and product quality of biopharmaceuticals. **D. Ponsi**, J. Purdie, D. Olson

9:10 BIOT **72.** Investigating the cause of charge variant shift of a monoclonal antibody from a mammalian cell culture process. **J. Cacciatore**, J. Weng, D. Mitchell, R. van Houts, J. van de Lagemaat, A.G. Tulloch, V. Janakiraman

‡ *Cooperative Cosponsorship*

9:30 BIOT **73.** Enabling product quality-driven development of cell culture processes for knobs-in-to-holes bispecifics. **J. Wuu**

9:50 Intermission.

10:10 BIOT **74.** Culture media influenced the phenotypic stability of an NS0 cell line—A case study. **T. Bui**, M. Berge, L. Li

10:30 BIOT **75.** Production of recombinant adenovirus in a single use bioreactor system. **G. Ahlén**, M. Bennemo, T. Persson, M. Lundgren

10:50 BIOT **76.** Reducing variability in cell specific productivity in perfusion culture. **Y. Shimoni**

11:10 BIOT **77.** Impact of gas entrance velocity on cell culture performance at small scale and manufacturing scale bioreactors: A case study. **M. George**, J. Tressel, B. Vincent, J. Ravikrishnan, A. Chhibbar, J. Cuenca, W. Asprec, H. Lin

Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Disruptive Bioprocessing & Process Integration

R. Barros, M. Brower, V. Natarajan, N. Tugcu, *Organizers*

M. Brower, S. M. Cramer, *Presiding*

8:30 BIOT **78.** Development of an integrated, automated, multi-product platform for the rapid production and purification of protein therapeutics. **L. Crowell**, N. Mozdzierz, A. Lu, A. Stockdale, K.R. Love, J.C. Love

8:50 BIOT **79.** Optimization of multi-column format for continuous capture of monoclonal antibodies. **S. Chollangi**, J. Angelo, D. Baur, X. Xu, N. Singh, M. Morbidelli

9:10 BIOT **80.** Streamlining biopharmaceutical decision-making: Designing for manufacturability, facility fit and cost-effectiveness. **S.S. Farid**

9:50 Intermission.

10:10 BIOT **81.** Design and control of integrated chromatography column sequences. **B. Nilsson**, N. Andersson, P. Tiainen, K. Köhler Van Alstine, A. Staby

10:30 BIOT **82.** Linking single pass tangential flow filtration with anion exchange chromatography for intensified mAb processing. **T. Elich**, E.M. Goodrich, H. Lutz, U. Mehta

10:50 BIOT **83.** Integrated continuous processing of proteins expressed as inclusion bodies: GCSF as a case study. **N. Kateja**, H. Agarwal, V. Hebbi, A.S. Rathore

11:10 BIOT **84.** Connected DSP mindset: How development enables future manufacturing visions. **L.W. Pampel**, R. Rodrigues, F. Gillet, M. Goebel, J. Shultz

Section C

InterContinental San Francisco

Union Square

Biophysical & Biomolecular Processes

Protein Structure & Function

J. Moore, J. A. Van Deventer, *Organizers*

H. Samra, T. Whitehead, *Presiding*

8:30 BIOT **85.** Molecular recognition of diverse type of odorants in a broadly tuned receptor OR2W1. **L. Ahmed**, V.S. Batista

8:50 BIOT **86.** Recon 3D: A resource enabling a three-dimensional view of human metabolism and disease. **E.C. Brunk**, S. Sahoo, D. Zielinski, A. Altunkaya, N. Mih, A. Prlic, A. Sastry, G. Gonzalez, A. Danielsdottir, A. Noronha, M. Aurich, P. Rose, R. Fleming, A. Draeger, S. Burley, J. Nielsen, I. Thiele, B.O. Palsson

9:10 BIOT **87.** Engineering enzymes for broad temperature range applications through active site flexibility. W. Wang, S. Dassetty, S. Sarupria, **M.A. Blenner**

9:30 BIOT **88.** Effect of co-solutes on viscosity and structure of highly concentrated monoclonal antibodies. **J. Hung**, B. Dear, A. Sharma, C. Karouta, M. Nieto, T. Truskett, K.P. Johnston

9:50 Intermission.

10:10 BIOT **89.** Efficient antibody affinity maturation requires co-selection of compensatory mutations to maintain thermodynamic stability. **M. Julian**, L. Li, S. Garde, P.M. Tessier

10:30 BIOT **90.** Non-destructive in-situ method for measuring protein concentration in frozen drug substance. **A. Borwankar**, C. Du, N. Singh

10:50 BIOT **91.** Functional and structural analysis of challenging protein targets using conformationally selective recombinant Fabs. **C. Craik**

Section D

InterContinental San Francisco

Telegraph Hill

Bio-Based Products

Engineering Microbes to Utilize Next Generation Feedstocks

M. R. Antoniewicz, C. A. Eckert, G. Sriram, *Organizers*

N. R. Boyle, C. Johnson, *Presiding*

8:30 BIOT **92.** Biological conversion of gaseous alkenes to liquid chemicals. **A. Case**

8:50 BIOT **93.** Bioconversion of natural gas: Commercially attractive gas to liquids technology. **B. Yeh**, C. Bodarky

9:10 BIOT **94.** Bioconversion of volatile fatty acids derived from waste activated sludge into lipids by *Cryptococcus curvatus*. **J. Liu**, J. Liu, M. Yuan, X. Huang

9:30 BIOT **95.** One-pot bioconversion of distiller dried gains hydrolysate to advanced biofuels. **F. Liu**, W. Wu, M.B. Tran-Gyamfi, R.W. Davis

9:50 Intermission.

10:10 BIOT **96.** Lactic acid production from the pyrolytic sugar levoglucosan. S.M. Rothstein, **T.J. Mansell**

10:30 BIOT **97.** Discovery of CO2-fixing one-carbon (C1) metabolism in a cellulose degrading bacterium *Clostridium thermocellum*. W. Xiong, P. Lin, L. Magnusson, L. Warner, J.C. Liao, P. Maness, **K.J. Chou**

10:50 BIOT **98.** Consolidating pretreatment and hydrolysis with engineered microbial consortia. **J. Henske**, S. Wilken, M.A. O'Malley

11:10 BIOT **99.** Photosynthetic production of butyrate: A versatile chemical and non-toxic alternative for butanol in cyanobacteria. **M.C. Lai**, E.I. Lan

Section E

InterContinental San Francisco

InterContinental B

Startup Road

Bioprocessing & Industrial Biotechnology

G. Bolton, A. May, T. Meyerrose, *Organizers*

A. Boesch, V. Mahendroo, T. Ransohoff, *Presiding*

8:30 BIOT **100.** Next generation process development: Stop experimenting. GoSilico. **T. Huuk**, T. Beck, T. Hahn, J. Hubbuch

8:50 BIOT **101.** Apeel sciences: Peels good! . **L. Perez**, C. Vild, M. Kahlscheuer

9:10 BIOT **102.** Puridify: Purifications solutions for biotherapeutic manufacturing. **O. Hardick**, I. Roberts

9:30 Intermission.

9:50 BIOT **103.** Tale of two companies: Comparing the founding and early growth of Sutro BioPharma and GreenLight Biosciences. **J.R. Swartz**

10:30 Panel Discussion.

Section F

InterContinental San Francisco

Sutter

Emerging Technologies

New Tools & Approaches: Cellular & Microbiome Engineering

Y. Y. Chen, Y. Kim, J. P. Pieracci, *Organizers*

H. Victor, *Organizer, Presiding*

Z. Shao, *Presiding*

8:30 BIOT **104.** Novel platform for the production of proteoglycans. **A. Roulier**, M. Kipper, C.A. Peebles

8:50 BIOT **105.** Tracking dual signal mediated antibiotic resistance transfer in *Enterococcus faecalis*. **A. Bandyoapdhyay**, P. Agrawal, R. Breuer, A. Barnes, D. Manias, K.D. Dorfman, G. Dunny, W. Hu

9:10 BIOT **106.** Phylogenetic and targeted functional profiling of the microbiome associated with a unique phytoremediation system. **J. Ravichandar**, A. Dyson, C.H. Collins

9:30 BIOT **107.** Elucidating physiology of microbial communities through co-culture 13C-metabolic flux analysis. **M.R. Antoniewicz**

9:50 Intermission.

10:10 BIOT **108.** Enhancing *Agrobacterium* mediated transient recombinant protein production in *Nicotiana benthamiana* plant cell suspension culture. **S. Sukenik**, K. McDonald

10:30 BIOT **109.** Developing microbiome-bots to treat inborn errors of metabolism. **Z. Mays**, N.U. Nair

10:50 BIOT **110.** Programmable control of CRISPR-Cas9 systems by engineering sgRNA as toehold-switchable riboregulators. **K. Siu**, W. Chen

11:10 BIOT **111.** Whole cell biosensor for detection and directed evolution of human milk oligosaccharide production. F. Enam, **T.J. Mansell**

Section G

InterContinental San Francisco

Grand Ballroom B/C

James M. Van Lanen Distinguished Service Award & Marvin J. Johnson Award in Microbial & Biochemical Technology

M. A. O'Malley, T. M. Przybycien, V. Roy, *Organizers*, *Presiding*

11:30 BIOT **112.** Building complex protein functions at the intersection of nanofabrication and synthetic biology. **W. Chen**

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Cellulose Structure & Biosynthesis

Mechanism of Synthesis

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

MONDAY AFTERNOON

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Control of Product Quality Attributes

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

Y. Cho, *Organizer, Presiding*

M. Mun, *Presiding*

2:00 BIOT **113.** Confessions of a cell culture engineer: Process impact on protein products in a quality-by-design world. **R.D. Kiss**

2:40 BIOT **114.** Modulation of the afucosylation level of recombinant antibodies with small molecule fucostatin inhibitors in cell culture processes. **J. Huang**, M. Mujacic, T. Hwang, O.R. Thiel, E. Le, J.G. Allen

TECHNICAL PROGRAM

3:00 BIOT **115.** Glycoengineering to improve biotherapeutic quality from CHO cells. **C. Chung**, B. Yin, S. Yang, Q. Wang, H. Zhang, M.J. Betenbaugh

3:20 Intermission.

3:40 BIOT **116.** Investigation into the cause of observed differences in the charge variants of a monoclonal antibody during production bioreactor process characterization studies. **N. Agarwal**, J. Kemper, A. Agarwal, J. Reier, J. Wang, S. Ahuja, G. Miro-Quesada

4:00 BIOT **117.** Control and estimation of glycosylation profile via media supplementation based on intracellular metabolic models in mammalian cell cultures. **S. Sha**, S. Yoon

4:20 BIOT **118.** Cathepsin D knockout in CHO cells using CRISPR/Cas9. **J. Baik**, K. Lee

4:40 BIOT **119.** Novel control strategy for pink colored IgG4 caused by vitamin B12. **C. Du**, R. Martin, Y. Huang, A. Borwankar, N. Singh, M.C. Borys, Z. Li

Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Disruptive Bioprocessing & Process Integration

R. Barros, M. Brower, V. Natarajan, N. Tugcu, *Organizers*

S. M. Cramer, *Organizer, Presiding*

M. Brower, *Presiding*

2:00 BIOT **120.** Chromatography-box-device for process-scale bio-separations. **R. Ghosh**

2:20 BIOT **121.** Continuous downstream purification with an all membrane process: Protein A capture and AEX flowthrough. **A. Gospodarek**, M. Brower, G. Skarja, D.J. Pollard

2:40 BIOT **122.** Engineering the calcium-regulated -roll peptide for bioseparations applications. **S. Banta**

3:00 BIOT **123.** Fit-for-purpose cGMP compliant magnetic separation device: Cleaning validation and protein purification results. **M. Ebeler**, M. Franzreb

3:20 Intermission.

3:40 BIOT **124.** Integration of ATPS and precipitation in a monoclonal antibody manufacturing process: The future of downstream processing? **F. Rudolph**, M. Richter, M. Dieterle, J. Studts

4:00 BIOT **125.** Exploring the limits of clarifying high cell density feeds with Cadence™ acoustic separator. **M. Collins**, K. Galipeau, E. Ayturk

4:20 BIOT **126.** Implementation of single-pass tangential flow filtration for inline concentration and production of drug substance: Module effects and diafiltration. **J. Zhang**, A. Arunkumar, N. Singh

4:40 BIOT **127.** Combining cell removal and Protein A affinity separation in the same unit operation. **I. Roberts**, C. Morris, M. Townsend

Section C

InterContinental San Francisco

Union Square

Biophysical & Biomolecular Processes

Protein Structure & Function

J. Moore, J. A. Van Deventer, *Organizers*

H. Samra, *Organizer, Presiding*

T. Whitehead, *Presiding*

2:00 BIOT **128.** Engineering a GPCR for biophysical analysis of oligomer interactions. **N.S. Schonenbach**, J. Yoo, A.M. Duran, M.D. Rieth, J. Meiler, S. Han, M.A. O'Malley

2:20 BIOT **129.** Withdrawn.

2:40 BIOT **130.** Saturation mutagenesis panning libraries enable activity and specificity modulation of Microcin J25. **S. Ritter**, Y. Kaznessis

3:00 BIOT **131.** Design and analysis of bioengineered models of Alzheimer's disease. **L.M. Walker**, J.B. Leach

3:20 Intermission.

3:40 BIOT **132.** Characterization of knobs-into-holes antibody assembly variants reveals structural plasticity in IgG Fc structure. **V. Lundin**, H. Zhang, A. Estevez, X. Guo, K. Lin, K. Tschudi, K. Catherman, F. Herrmann, J. Quang, K. Aurori, J. Giulianotti, M. Bhaumik, A. Ladiwala, H. Liu, J. Zhang, C. Ciferri, J. Shimoni-Zhu

4:00 BIOT **133.** Effect of protein-stabilizer microheterogeneity on long-term stability in solid-state biopharmaceutical formulations. **S.H. Koshari**, K. Rajagopal, I.E. Zarraga, Y. Liu, N.J. Wagner, A.M. Lenhoff

4:20 BIOT **134.** Process linkage experiments to support the design space of a biopharmaceutial manufacturing process. **N.L. McKnight**, K. Lazzareschi, R. St. John, B.D. Kelley

4:40 BIOT **135.** Effective virus clearance using strong anion exchange bind/elute chromatography. **M. Garcia**, R. Specht

Section D

InterContinental San Francisco

Telegraph Hill

Bio-Based Products

Facility Enabled Opportunities

C. A. Eckert, G. Sriram, *Organizers*

M. R. Antoniewicz, *Organizer, Presiding*

Y. Yoshikuni, *Presiding*

2:00 BIOT **136.** Opportunities for facility-enabled science at the DOE Joint Genome Institute (JGI). **Y. Yoshikuni**

2:20 BIOT **137.** DOE Environmental Molecular Sciences Laboratory: Accelerating biological research for biobased product production. **J. Evans**, S.E. Baker

2:40 BIOT **138.** Genomic and transcriptomic analysis of *Rhodosporidium toruloides* producing biofuels from depolymerized polysaccharides and lignin. **J. Kim**, Y. Junko, M. Reilly, B.A. Simmons, J.K. Magnuson, J.M. Skerker, J.M. Gladden

3:00 BIOT **139.** Parts list for fungal cellulosomes revealed by proteomics and comparative genomics. **S. Gilmore**, C.H. Haitjema, J. Henske, K. Solomon, R. de Groot, A. Kuo, S.J. Mondo, A.A. Salamov, K. LaButti, H.M. Brewer, S.O. Purvine, A.T. Wright, S.E. Baker, I.V. Grigoriev, M.A. O'Malley

3:20 Intermission.

3:40 BIOT **140.** Comparison of base-catalyzed depolymerization of lignin sourced from multiple biochemical conversion processes, biomass sources, and feedstock processing processes. **R. Katahira**, X. Chen, E.M. Kuhn, M.P. Tucker, G. Beckham, A.E. Ray, N. Nagle

4:00 BIOT **141.** Exploring the functional landscape of aldehyde deformylating oxygenase activity throughout the ferritin superfamily. **J.B. Siegel**

4:20 BIOT **142.** Biocatalysis with flavin-dependent halogenases for selective C-H functionalization. **M. Andorfer**, J.C. Lewis

4:40 BIOT **143.** Urease Crosslinked Enzyme Lyophilizates (CLELs) streamlining conventional organic syntheses. **T. Akkas**, A. Zakharyuta

Section E

InterContinental San Francisco

InterContinental B

Startup Road

Diagnostics, Devices, New Therapeutic Modalities & Personalized Medicine

G. Bolton, A. May, T. Meyerrose, *Organizers*

S. Flaim, S. Gallant, L. Lu, *Presiding*

2:00 BIOT **144.** SimpleScan platform for rapid, quantitative, multiplexed and fully automated protein assays for pharma and diagnostic applications. K. Araz, S. Tia, **A. Apori**

2:20 BIOT **145.** Host-response biomarkers: A disease-defining diagnostic for sepsis. **T.E. Sweeney**, P. Khatri

2:40 BIOT **146.** Utilizing the skin microbiome for UV protection- Can a startup do it? . **N. Qvit-Raz**

3:00 BIOT **147.** Advanced glycation end products as predictors of diabetic complications. **P.J. Beisswenger**

3:20 Intermission.

3:40 BIOT **148.** Xip: From idea to impact in IVD. **O. Florescu**, T. Siegel

4:00 Panel Discussion.

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Cellulose Structure & Biosynthesis

Synthase Trafficking & Synthesis of plant (1->3),(1->4)-D-glucans

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Undergraduate Research Posters

Biotechnology

Sponsored by CHED, Cosponsored by BIOT and SOCED

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

M. A. O'Malley, V. Roy, *Organizers*

8:00 - 10:00

237, 239, 249-250, 264, 273, 279, 297, 305, 312, 326, 334, 346, 349, 352, 364, 378, 385, 390, 392, 480, 581. See subsequent listings.

TUESDAY MORNING

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Microbial & Non-Model Hosts: Strain Engineering & Process Development

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

K. Solomon, K. Veeravalli, *Presiding*

8:30 BIOT **149.** Developing the thermotolerant yeast *Kluyveromyces marxianus* as a microbial host for volatile ester biosynthesis. A. Loebs, R. Engel, C. Schwartz, **I.R. Wheeldon**

8:50 BIOT **150.** Extremely thermophilic organisms for efficient glucose and xylose fermentations. **M.R. Antoniewicz**

9:10 BIOT **151.** Improved production of biochemicals and biofuels with reduced CO2 emissions. **S. Jones**, B.P. Tracy, J.R. Phillip, P.C. Munasinghe

9:30 BIOT **152.** Retroelements for continuous evolution. **A.J. Simon**, A.T. Tucker, B.W. Davies, A.D. Ellington

9:50 Intermission.

10:10 BIOT **153.** Sugar sensors and transporters in biomass-degrading anaerobic fungi. **S. Seppala**, I. Podolsky, J. Yoo, D. Yur, M.A. O'Malley

10:30 BIOT **154.** Enabling glucose-xylose co-utilization in yeast through expression of xylose-specific transporters. **M. Gao**, M. Cao, Q. Su, Z. Shao

10:50 BIOT **155.** Engineering photosynthetic production of L-lysine. **T. Korosh**, **A.L. Markley**, R. Clark, B. Pfleger

11:10 BIOT **156.** Development of a general defined media for *Pichia pastoris* protein expression. **M. Bartlett**, K.R. Love, J. Clark, A. Kuo, A. Roberts, J.C. Love

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

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Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Antibodies, Drug Conjugates & Novel Formats

R. Barros, V. Natarajan, N. Tugcu, *Organizers*

A. Ladiwala, M. A. Rito Palomares, N. Sanaie, *Presiding*

8:30 BIOT **157.** Process control to minimize product related conjugation variants in the manufacture of ADCs. **D. Olson**, R. Hendricks, M. Hutchinson, R.L. Beardsley

8:50 BIOT **158.** Mechanistic model of excipient exchange during protein UF/DF. **J. Ladwig**, R. Hart

9:10 BIOT **159.** Downstream process development and scale-up for *Streptoverticillium* transglutaminase expressed in *E.coli,* and its application to enable site-specific conjugation in ADC production. **S. Chen**, W. Wellborn, J. Cundy, B. Chen, E. Barr, L. Determan, B. Nolting, J. Martin

9:30 BIOT **160.** Mechanism and application of dextran sulfate in protein A affinity chromatography to achieve improved HCP and DNA clearance for biologics purification. **C. Huang**, J. Angelo, X. Xu, Z. Li

9:50 Intermission.

10:10 BIOT **161.** Thermo-separating polymer-based aqueous two-phase systems for the fractionation and recovery of PEGylated lysozyme species. G. Hernández-Vargas, M. González-González, M.A. Rito Palomares, **J. González-Valdez**

10:30 BIOT **162.** High viscosity tangential flow filtration applications: The impact of feed channel screen on process performance, high concentration capability, and membrane re-use. **D. Kinzlmaier**, E.M. Goodrich

10:50 BIOT **163.** Downstream process development considerations to address polysorbate degradation in drug substance formulation. **Y. Yigzaw**, A. Morris, M. Sawant, J. Gu

11:10 BIOT **164.** Continuous in line flocculation, new opportunities for primary separation and economic impact. **P. Satzer**, D. Burgstaller, W. Krepper, A. Cataldo, J. Haas, M. Maszelin, J. Mohoric, K. Pajnic, A. Jungbauer

Section C

InterContinental San Francisco

Union Square

Biophysical & Biomolecular Processes

Prediction & Characterization of Biophysical Properties

J. Moore, J. A. Van Deventer, *Organizers*

S. Kumar, P. Tamamis, *Presiding*

8:30 BIOT **165.** Structure of concentrated antibody solutions in the presence of weak self-association. **D. Corbett**, C. Avendaño, M. Hebditch, C. van der Walle, S. Uddin, R. Curtis

8:50 BIOT **166.** Effects of thermal-stress and glycan-removal on structural integrity of a human IgG1 antibody: Insights from extended molecular dynamics simulations. **D. Tomar**, S. Kumar, S. Singh

9:10 BIOT **167.** Towards predictive models of antibody biophysical properties and aggregation. **G. Ferreira**, H. Samra, R.L. Remmele, C.J. Roberts

9:30 BIOT **168.** Semiempirical and quantum chemical prediction of ATP affinities and non-covalent binding to P-loops of proteins. **J.H. Rodriguez**

9:50 Intermission.

10:10 BIOT **169.** Signaling protein diffusion and accurate molecular weight based estimations of biomolecule dynamics. **C.J. Fennell**, N. Ghousifam, H. Gappa-Fahlenkamp

10:30 BIOT **170.** Withdrawn.

10:50 BIOT **171.** Time-resolved anisotropy measurements of single, non-tethered tau proteins in solution. **A. Foote**, L. Manger, R.H. Goldsmith, M.R. Holden, M. Margittai

11:10 BIOT **172.** Recent advances in affinity maturation with the ADAPT platform. **T. Sulea**, C.R. Corbeil, E.O. Purisima

Section D

InterContinental San Francisco

Telegraph Hill

Bio-Based Products

Synthetic Biology & Metabolic Engineering using Omics Based Approaches

M. R. Antoniewicz, C. A. Eckert, G. Sriram, *Organizers*

J. L. Avalos, T. Lee, *Presiding*

8:30 BIOT **173.** Reverse engineering of short-chain fatty acid tolerance and production in *E.coli*. **Y. Chen**, E. Boggess, J. Shanks, T. Mansell, J. Dickerson, L.R. Jarboe

8:50 BIOT **174.** Production of acyl esters and its analogous from microbes. **W. Kim**, Z. Guo, O. Zelder, G.V. Abendroth

9:10 BIOT **175.** Designing aptazyme-based biosensor delay control systems to minimize expression-associated stresses in engineered biosynthetic pathways. **J. Stevens**, J.M. Carothers

9:30 BIOT **176.** Characterizing *in vivo* isopentenyl diphosphate (IPP) toxicity in isoprenol-producing *E. coli*. K.W. George, M. Thompson, **J. Kim**, E. Baidoo, C.J. Petzold, J.D. Keasling, **T. Lee**

9:50 Intermission.

10:10 BIOT **177.** Evolution of biomass-degrading anaerobic consortia revealed by metagenomics. **X. Peng**, S. Gilmore, J. Henske, C. Swift, M. Theodorou, D.L. Valentine, M.A. O'Malley

10:30 BIOT **178.** Flux coupling analysis for studying the dependencies and degrees of freedom in thermodynamically constrained metabolic network models. **Z. Hosseini**, M. Ataman, N. Hadadi, V. Hatzimanikatis

10:50 BIOT **179.** Omics-enabled discovery of a novel bacterial enzyme, phenylacetate decarboxylase, enabling bio-based toluene production. **H.R. Beller**, A. Rodrigues, K. Zargar, A. Saini, S. Tringe, J.D. Keasling, C.J. Petzold

11:10 BIOT **180.** Bio-based products: Synthetic biology approaches to engineer production of biofuels & value-added chemicals. **C.J. Harvey**, M. Teng, J. Horecka, U. Schlecht, C. Fischer, M. Miranda, J. Cherry, R. Davis, R. St. Onge, Y. Tang, M. Hillenmeyer

Section E

InterContinental San Francisco

InterContinental B

Downstream Processes

Automated Technologies & High Throughput Systems in Biologics Production

R. Barros, V. Natarajan, N. Tugcu, *Organizers*

M. Ottens, J. Pollard, *Presiding*

8:30 BIOT **181.** Overcoming limitations of high throughput scale chromatography columns to facilitate the evaluation of extended resin lifetime. **C. Andersen**, G. Bolton, H. Hoang

8:50 BIOT **182.** High throughput process development application in the DoE study of insulin analog capture step. S. Liao, D. Wu, **B. Wang**

9:10 BIOT **183.** Integration of downstream platform development into a single 96-well filter plate for ultra-rapid process definition. **R. Gillespie**, M. McClure, S. Freeman, L. Connell-Crowley

9:30 BIOT **184.** Development of a high-throughput microscale cell disruption platform for *Pichia pastoris* in rapid fermentation process design. **B. Blaha**, T. Mukhopadhyay

9:50 Intermission.

10:10 BIOT **185.** Miniaturized techniques for high throughput biopurification process development. **M. Ottens**

10:30 BIOT **186.** Rapid determination of partition coefficients of biomolecules in a microfluidic ATPS platform using fluorescence microscopy. **R. Aires-Barros**, D. Silva, A. Azevedo, P. Fernandes, V. Chu, J. Conde

10:50 BIOT **187.** Utilizing fluidized bed resin tips for high-throughput clarification and capture. **M. Rauscher**, J. Pollard, J.P. Welsh, M. Manahan, N. Tugcu

11:10 BIOT **188.** Integrated precipitation and periodic counter-current chromatography process. **S. Grosshans**, G. Wang, P. Baumann, J. Hubbuch

Section F

InterContinental San Francisco

Sutter

Emerging Technologies

New Tools & Approaches: Molecular & Biochemical Technologies

Y. Y. Chen, Y. Kim, L. Morsut, J. P. Pieracci, *Organizers*

L. Morsut, S. Ozturk, *Presiding*

8:30 BIOT **189.** Rational design and study of polysialic acid-binding peptides. **D. Shastry**, P. Karande

8:50 BIOT **190.** Enhancing the chemical versatility and throughput of yeast display. H.P. Kehoe, C.E. Ghadban, J.T. Stieglitz, L.B. Quinto, J.B. Lissoos, **J.A. Van Deventer**

9:10 BIOT **191.** Rewiring genome structure with programmable CRISPR-Cas tools to physically reposition genes. **J. Zalatan**

9:30 BIOT **192.** Controlled protein degradation for the conditional survival of cancer suicide enzymes. **A. Gaynor**, W. Chen

9:50 Intermission.

10:10 BIOT **193.** High throughput analysis of the antibody specificity repertoire for antigen identification and diagnostic applications. **J. Bozekowski**, M.L. Paull, P. Daugherty

10:30 BIOT **194.** Covalent trapping reveal that phosphorylated EGFR oligomers activate Ras more potently than dimers. **Z. Gartner**, S. Liang, D. Patterson

10:50 BIOT **195.** Accelerated biomolecular kinetics revealed by microdroplet fusion mass spectrometry. **J. Lee**, H. Nam, R.N. Zare

11:10 BIOT **196.** Highly sensitive and selective peptide-based fluorescent probe for Endoplasmic Reticulum Aminopeptidase Associated with Antigen Processing (ERAAP). **J. Zhang**, S. Yang, F. Gonzalez, N. Shastri, N. Murthy

Section G

InterContinental San Francisco

Grand Ballroom B/C

W. H. Peterson Awards & BIOT Young Investigator Award

M. A. O'Malley, T. M. Przybycien, V. Roy, *Organizers*, *Presiding*

11:30 BIOT **197.** Repurposing ribosomes for synthetic biology. **M.C. Jewett**

Cellulose Structure & Biosynthesis

Biochemistry & Cellular Biology

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of David R. Walt

Sponsored by ANYL, Cosponsored by BIOT

TUESDAY AFTERNOON

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Metabolic Engineering & Synthetic Biology

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

J. Latone, T. J. Mansell, *Presiding*

2:00 BIOT **198.** Engineering and modeling of a modular, motility-based biosensor system in Escherichia coli. **J. Ravichandar**, A. Bower, A. Julius, C.H. Collins

2:20 BIOT **199.** Development and demonstration of a robust and scalable two-stage fermentation system for enhanced bioproduction. **Z. Ye**, M. Lynch

2:40 BIOT **200.** Exploring chemodiversity in metabolism towards the integration of chemistry into biology. **J. Hafner**, **N. Hadadi**, V. Hatzimanikatis

3:00 BIOT **201.** Metabolic engineering of bacteria for production of oleochemicals. N. Hernandez, M.J. Grisewood, C. Maranas, **B. Pfleger**

3:20 Intermission.

3:40 BIOT **202.** Metabolic flux analysis of transgenic *E. coli* BL21(DE3) producing a non-specific antivenom. **I. Sawaya**, C.F. Komives

4:00 BIOT **203.** Genetic system for regulatory sRNA retargeting and scaffold optimization: Metabolic engineering applications. **R.A. Lease**, A. Lahiry, S.D. Stimple, D.W. Wood

4:20 BIOT **204.** Systems biology approaches for engineering microbial biocatalysts. **J. Reed**

Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Antibodies, Drug Conjugates & Novel Formats

R. Barros, V. Natarajan, N. Tugcu, *Organizers*

A. Ladiwala, M. A. Rito Palomares, N. Sanaie, *Presiding*

2:00 BIOT **205.** Development of adsorptive hybrid filters to enable two-step purification of biologics. **A. Arunkumar**, N. Singh, M. Peck, A. Voloshin

2:20 BIOT **206.** Process development for the enzyme-mediated manufacture of site-specific ADCs for early clinical trials. **B. Nolting**

2:40 BIOT **207.** Optimization of process parameters for viral filtration of therapeutic monoclonal antibodies. **H. Tjandra**, R. Zolyomi, G. Prakash, D. Surendar, K. Shill, Y. Chang, X. Pan, T. Luong, A. Hesslein

3:00 BIOT **208.** Innovative Hydrophobic Interaction Chromatography (HIC) resins for next generation molecule challenges. **O. Terova**

3:20 Intermission.

3:40 BIOT **209.** High resolution experimental design to study antibody-drug conjugation process robustness. **B. Sackett**, T. Peram, J. Franklin

4:00 BIOT **210.** Direct demonstration of scalability of virus removal filter performance. **B. Buesing**, D. Strauss, A.H. Schwartz, T. Miyabayashi, N. Hirotomi

4:20 BIOT **211.** Platform approach to purification of albumin-fusion proteins. **T.M. Pabst**, C. Thompson, M. Fonseca, A.K. Hunter, X. Wang, L. Tie

4:40 BIOT **212.** Protein A chromatography as capture step for antibody fragments: Mechanism of interaction and case study. **G. Platteau**, G. Ströhlein, B. Van der Jeugt, G. Lissens, V. Gasparlunaite, S. Muyldermans, C. Vincke, Y. Sterckx

Section C

InterContinental San Francisco

Union Square

Biophysical & Biomolecular Processes

Protein Interactions & Interfaces

J. Moore, J. A. Van Deventer, *Organizers*

S. Kumar, P. Tamamis, *Presiding*

2:00 BIOT **213.** Toolbox of experimental and *in silico* methods to predict protein long-term stability. **M. Schermeyer**, P. Baumann, J. Hubbuch

2:20 BIOT **214.** Predicting the structure and orientation of adsorbed peptides with molecular simulations. **K. Sprenger**, T. Weidner, F. Baneyx, J. Pfaendtner

2:40 BIOT **215.** Coupling experiment and modeling to understand peptide capture agent specificity for similar protein targets. **D.A. Sarkes**, M. Hurley, D.N. Stratis-Cullum

3:00 BIOT **216.** Aggregation kinetics for IgG1-based monoclonal antibody therapeutics. **R. Bansal**, A. Singla, V. Joshi, A.S. Rathore

3:20 Intermission.

3:40 BIOT **217.** Extractables studies on single-use components in the manufacture of Antibody Drug Conjugates (ADCs). **K. Isaksson**, S. Burke, A. Graanberg, F. Lundstrom

4:00 BIOT **218.** Site-selective approach for DNA directed immobilization of enzymes via oxidative coupling. **T. Hurlburt**, K. Palla, M.B. Francis, G.A. Somorjai

4:20 BIOT **219.** Noncovalent modulation of protien energy landscapes with an emerging class of cyclic-peptide chaperones. **D.N. Bunck**, B. Atsavaprannee, K. Museth, J.R. Heath

4:40 BIOT **220.** Enzyme-Polymer conjugates. Improving the activity of cellulase for biofuel applications. **D. Konkolewicz**, R.C. Page, M. Lucius, T. Wright, H. Fischesser, J. Shepherd, J. Stewart

Section D

InterContinental San Francisco

Telegraph Hill

Bio-Based Products

Synthesis in Space

M. R. Antoniewicz, C. A. Eckert, G. Sriram, *Organizers*

M. A. Blenner, M. Roberts, *Presiding*

2:00 BIOT **221.** Bio-based synthesis on the International Space Station U.S. National Lab. **M. Roberts**

2:20 BIOT **222.** Materials processing on the International Space Station and enabling long-term industry access to low Earth orbit. **J.A. Robinson**, K. Costello

2:40 BIOT **223.** Microgravity biologics crystallization processes. **P. Reichert**

3:00 BIOT **224.** X-ray and neutron crystallographic structures of Inorganic pyrophosphatase determined from microgravity-grown crystals. **J.D. Ng**, J.M. Garcia-Ruiz

3:20 Intermission.

3:40 BIOT **225.** Methane metabolism by yeast for solar system exploration. A. Rahman, M.J. Dougherty, J.A. Hogan, **J.M. Galazka**

4:00 BIOT **226.** Synthetic biology for recycling human waste into nutraceuticals and materials. D. Gao, M. Spagnuolo, G. Rodriguez, M. Brabender, K. Scola, **M.A. Blenner**

4:20 BIOT **227.** Engineering cyanobacteria for the conversion of CO2 to lightweight materials. **F. Zhang**, S. Rommelfanger, Y. Xiao

4:40 Panel Discussion.

Section E

InterContinental San Francisco

Sutter

Emerging Technologies

Precision Medicine: Biomarkers & Targeted Therapeutics

Y. Y. Chen, B. Hackel, Y. Kim, J. P. Pieracci, *Organizers*

D. Liu, C. Pirie, *Presiding*

2:00 BIOT **228.** Designing targeted therapeutics to interrogate intracellular tumor antigens. **P. Ho**, C. Ede, Y.Y. Chen

2:20 BIOT **229.** Prodrug activation controlled by Boolean logic-gated nucleic acid strand displacement inside live cancer cells. **R.P. Chen**, W. Chen

2:40 BIOT **230.** MicroRNA-Triggered dCas9 binding to a molecular beacon for cancer detection. **L. Dorsey**, R.P. Chen, W. Chen

3:00 BIOT **231.** Raman molecular urinalysis. **R.S. Senger**, J. Robertson

3:20 Intermission.

3:40 BIOT **232.** Volatile organic compounds in breath associated with hypoglycemia in type 1 diabetes. **A. Siegel**, A. Daneshkhah, D.S. Hardin, K. Varahramyan, M. Agarwal

4:00 BIOT **233.** Human *in vivo* nanoparticle protein corona in ovarian carcinoma patients: A novel tool for biomarker discovery. **M. Hadjidemetriou**, K. Kostarelos

4:20 BIOT **234.** Rotaxane probes for applications in molecular detection with Xe hyperCEST NMR. **J. Finbloom**, C.C. Slack, C.J. Bruns, K. Jeong, D.E. Wemmer, A. Pines, M.B. Francis

4:40 BIOT **235.** Regulating immune tolerance using quantum dots to track and control the density of self-antigen display. K.L. Hess, E. Oh, I. Medintz, **C. Jewell**

TUESDAY EVENING

Section A

Moscone Center

West Hall

Poster Session

N. U. Nair, K. Solomon, *Organizers*

6:00 - 8:00

BIOT **236.** *In vitro* evaluation of folic acid-conjugated redox-responsive mesoporous silica nanoparticles for the delivery of cisplatin. ^**M.P. Alvarez**, J.L. Vivero-Escoto

BIOT **237.** Nonviral genome editing based on a CRISPR nanocomplex for target-specific treatment of multidrug-resistant bacterial infections. **Y. Kang**, H. Chung

BIOT **238.** New effective washing step in protein A purification. **O. Jensen**, P. Kærsgaard

BIOT **239.** Characterization and kinetics of fragmentation in IgG1 based monoclonal antibody products. **R. Bansal**, S. R., N. Chhabra, A.S. Rathore

BIOT **240.** Bioinspired dual-cross-linked tough protein hydrogel as a catalytic matrix for CO_2 sequestration. **C. Kim**, Y. Yang, H.J. Cha

BIOT **241.** Optimizing expression of tissue-type plasminogen activator in *E.coli*. **O. Vega**, **V. Torres Irizarry**, **V. Rodriguez Torres**, S. Chattopadhyay, **V. Bansal**

BIOT **242.** siRNA Delivery with hybrid collagen/cell penetrating peptide carriers. **A. Gamboa**, K. Slowinska

BIOT **243.** Investigating and understanding process improvements for transient production of virus like particles in HEK 293 cells. **D.J. Blackstock**, P. Chen, P. Biswas, J. Horwitz, R. Schwartz

BIOT **244.** Cytotoxicixty and acute toxicity studies of imidazolium-based ionic liquids. **W. Han**, Q. Chang, L. Li, B. Zhong, K. Yeung

BIOT **245.** Production of jet fuel precursor monoterpenoids from engineered *Escherichia coli*. **D. Mendez-Perez**, J. Alonso-Gutierrez, Q. Hu, M. Molinas, E. Baidoo, G. Wang, L. Chan, C.J. Petzold, P.D. Adams, J.D. Keasling, T. Lee

BIOT **246.** Impact of feed composition on protein A chromatography lifetime and residual foulants. **D.G. Bracewell**, K. Lintern, M. Pathak, A.S. Rathore

BIOT **247.** Conversion of biomass to value-added bioproducts by enzyme nanoassemblies. **C. Lee**, R. Kibblewhite, K.C. Wagschal

BIOT **248.** Enhanced galactosylation of a monoclonal antibody. R. Anderson, L. Hock, **S. Ozturk**, J. Yan

BIOT **249.** Silica shell/adhesive composite film for color Doppler ultrasound guided needle placement. **T. Sung**, J. Yang, J. Wang, E. Ward, N. Mendez, C. Barback, S. Blair, A. Kummel, W.C. Trogler

BIOT **250.** Investigation into thermodynamic binding mechanisms of protein-ligand interactions in MM chromatography using surface plasmon resonance. **R.B. Gudhka**, S. Ranjan, S. Banerjee, S.M. Cramer

BIOT **251.** Achieving desired monoclonal antibody product quality attributes throgh cell culture process manipulations. **M. Leith**, A. Chen

BIOT **252.** Coarse grained model development of enzymatic lignocellulosic biomass degradation by fungal cellulosomes. **S. Wilken**, M.A. O'Malley

BIOT **253.** Defining important protein surface property clusters to predict retention in multimodal chromatography systems. **J. Robinson**, C. Bilodeau, S.M. Cramer

BIOT **254.** Withdrawn.

BIOT **255.** mAb Aggregate removal using flow through chromatography on fractogel. **M. Dillingham**, O. Jensen, N. Laroudie

BIOT **256.** Enzymatic synthesis of DNA-RNA nanoparticles for efficient siRNA delivery. L. Jae Sung, J. Lee, **D. Kim**

BIOT **257.** Rapid, integrated purification process development for non-mAb biologics with variant challenges. **C. Goodwine**, S. Timmick, N. Vecchiarello, S.M. Cramer

BIOT **258.** Identifying and characterizing the secondary metabolites of anaerobic fungi. **C. Swift**, M.A. O'Malley, K. Louie, **T. Northern**

BIOT **259.** *In silico* process design tool for rapid identification of orthogonally selective multimodal chromatographic materials for HCP removal. **N. Vecchiarello**, S. Timmick, C. Goodwine, S.M. Cramer

BIOT **260.** Developing computational tools for understanding and predicting protein retention behavior in multimodal chromatographic systems. **C. Bilodeau**, S. Banerjee, S. Garde, S.M. Cramer

‡ *Cooperative Cosponsorship*

BIOT **261.** Process analytical technology for the rapid quantitation of underivitized amino acids in bioreactor media by mass spectrometry. **D.N. Powers**, C. Agarabi

BIOT **262.** Feasibility of formulating a highly concentrated monoclonal antibody (mAb) into a buffer-free solution using tangential flow filtration (TFF). **W. Chang**, D. Chen, D. Laikijrung, X. Xin

BIOT **263.** Co-expression of Bacterial Microcompartment (BMC) shell proteins shield toxicity of lysis protein E from bacteriophage ΦX174 during recombinant expression in *E. coli*. **M.C. Yung**, F. Bourguet, T. Carpenter, M. Coleman

BIOT **264.** Mycoplasma clearance and risk analysis in a model bioprocess. **J. Wang**, M. Brown, A. Dabrazhynetskaya, V. Chizhikov, K.A. Brorson

BIOT **265.** Robust viral clearance on virus removal filters using a targeted virus spiking approach. **E. Vyas**, N. Takahashi, M. Burnham, P. Nemitz, D. Strauss, N. Hirotomi

BIOT **266.** Combinatorial strategies for optimizing polyketide production in *Saccharomyces cerevisiae*. **T. McTaggart**, N.A. Da Silva

BIOT **267.** Combinatorial engineering of the mevalonic acid pathway for optimization of valerena-1,10-diene production. **J. Tran**, J. Lamberts, S.P. McCormick, E. Nybo

BIOT **268.** Combinatorial enzymatic synthesis of lipid A analogs. **K. Sankar**, C. Khosla

BIOT **269.** Liposome-based co-delivery of paclitaxel and docetaxel enhances oxidative stress in MCF-7 breast cancer cells. **V. Geraldo**, I.M. Paino, F.L. Maccari, M. Scarpa, V. Zucolotto, O.N. Oliveira

BIOT **270.** Evaluation of single-use technologies for the primary clarification of pre-treated bacterial harvest feedstreams. **F. DiGennaro**

BIOT **271.** High throughput solubility screening for developability assessment during therapeutic antibody discovery. Q. Chai, **J.J. Shih**

BIOT **272.** Integration of near-IR spectroscopy in to bench-scale bioreactors. **B. Chavez**, S. Velugula, N. Trunfio, C. Agarabi, K.A. Brorson

BIOT **273.** Tracking single quantum dots to unravel membrane diffusion dynamics of the ADHD/autism/bipolar disorder-associated Ala559Val dopamine transporter coding variant. **L.B. Thal**, I.D. Tomlinson, R.D. Blakely, S.J. Rosenthal

BIOT **274.** Detection of LAMP amplified Amelogenin gene using a binary deoxyribozyme sensor. **A. Smith**

BIOT **275.** Optimization of protein A chromatography process for a Herceptin® biosimilar (trastuzumab). **A. Naresh**, C. Caroselli, W. Dendamrongvit, C. Yonan, D. Bailey, M. Siwak

BIOT **276.** Mussel-inspired waterproof protein glue for treatment of urinary fistula. **H. Kim**, H.J. Cha

BIOT **277.** Surface adhesion to cohesion switched by dopa-Fe3+ complexation in response to microenvironment at the mussel plaque-substrate interface. **B. Yang**, C. Lim, D. Hwang, H.J. Cha

BIOT **278.** Engineered zinc finger proteins immobilized on beads as a novel diagnostic application for detection of pathogen-specific DNA sequences. **B. Kim**, D. Kim, M. Kim

BIOT **279.** Development of a synthetic metabolic engineering tool for the yeast Yarrowia lipolytica. **K. Frogue**, C. Schwartz, M. Shabbir-Hussain, M.A. Blenner, I.R. Wheeldon

BIOT **280.** High-yield & high-speed biohydrogen production from starch and water via in vitro synthetic enzymatic pathways. **J. Kim**, Y. Zhang

BIOT **281.** Implementing single-use assemblies: Design qualification testing & implications. **A. Steele**

BIOT **282.** Structure-function studies of the *Thermodesulfovibrio yellostonii* ADP-Glucose Pyrophosphorlyase. **E. Yik**, S. Kaur, E. Pushkarev, E. Mercado, M. Collazo, D. Cascio, H. Axelrod, **C.R. Meyer**

BIOT **283.** Engineering characterization and cultivation of fast growing plant suspension cells using the ReadyToProcess WAVE™ 25 bioreactor system. **A. Castan**, S. Werner, M. Stalder, D. Eibl, R. Eibl

BIOT **284.** Case study: Impact of polishing step sequence order on the manufacturing of therapeutic monoclonal antibodies. **D. Surendar**, X. Pan, H. Tjandra, A. Hesslein

BIOT **285.** Investigation of barrier technologies for clearance of mycoplasma in bioprocess solutions. **S. Johnson**, **S. Lute**, M. Brown, S. Dolan, C. Breuning, K.A. Brorson

BIOT **286.** Secretion of functional formate dehydrogenase in *Pichia pastoris*. **M.P. Takacs**, O.V. Makhlynets, P.L. Tolbert, I.V. Korendovych

BIOT **287.** Monitoring directed evolution of enzymes with Raman spectroscopy. **A. Fisher**, D.R. Bevan, R.S. Senger

BIOT **288.** Withdrawn.

BIOT **289.** Recent advances in RNA centric tools that detect, visualize, and covalently modify specific RNAs in fixed and living tissues. **S.C. Alexander**, N.K. Devaraj

BIOT **290.** Characterization of chinese hamster ovary host cell protein interactions with monoclonal antibody by yeast surface display. C. McGovern, **K.M. Doolan**

BIOT **291.** Screening and partial characterization of moderate halophilic hydrolases with good stability in organic solvents. **E. Fasoli**, M. Matar Abed, J.J. Sanchez, **S. Toro**, I. Rivera, A. Miranda

BIOT **292.** Exploring protein-excipient interactions via on-column screening and complementary methods. R. Pirnie, **M.E. Krause**, M. Ogunyankin, F. Rinaldi, S. Patke, A.S. Narang, M.L. Adams, R.B. Gandhi

BIOT **293.** Role of metals in crosslinking of virus-like particles. **E. Wen**, J. Konietzko, J.G. Joyce, M. Kosinski

BIOT **294.** Clone selection and process development for recombinant HIV trimers. **P. Chen**

BIOT **295.** Investigating the effect of oxidation of granulocyte colony stimulating factor on biological activity using experimental and computational approach. **S. Singh**, A. Mishra, D. Kumar, A.S. Rathore

BIOT **296.** Assessing analytical comparability of biosimilars: GCSF as a case study. **N. Nupur**, S. Singh, G. Narula, A.S. Rathore

BIOT **297.** Electrical stimulation of human dermal fibroblasts and quantification of collagen, collagenase, and elastin with morphology studies. **E. Nguyen**, K. Columna, J. Wishner, K. Slowinska

BIOT **298.** Electrospining of bio-based polyurethane and its drug delivery properties. **H. Lv**, D. Tang, L. Zhang

BIOT **299.** Metabolic engineering of *Corynebacterium glutamicum* for the production of D-lactate and ethyl lactate from corn stover hydrolysates. **A. Varman**, J.M. Gladden, R.W. Davis

BIOT **300.** Position-Dependent screening of luminescence in flotation immunoassay. **H. Chen**, A. Hagstrom, J. Kim, G. Garvey, A. Paterson, F. Ruiz-Ruiz, B. Raja, U. Strych, M.A. Rito Palomares, K. Kourentzi, J. Conrad, R. Atmar, R.C. Willson

BIOT **301.** Characterization of mAB HMW and monomer species to enhance downstream process development. **H.R. Doss**, A. Shupe, R.K. Swanson, D. Wang, L. Chemmalil

BIOT **302.** End-to-end-process: From genetic engineering to chemical valorization of unsaturated fatty acids from microalgae. **S. Hess**, V. Goldbach, D. Ewe, S. Mecking, P. Kroth

BIOT **303.** Continuous processing of biotherapeutics through application of a novel Coiled Flow Inversion Reactor (CFIR). **N. Kateja**, H. Agarwal, A.S. Rathore

BIOT **304.** Automated atom-mapped metabolic network reconstruction of *E-coli* from *in silico* labeled metabolites. **J. Hafner**, N. Hadadi, V. Hatzimanikatis

BIOT **305.** Multi-objective flux analysis software for the COBRA toolbox. **M. Griesemer**, A. Navid

BIOT **306.** Silica nanostructured multilayer assembly using engineered mussel glue for accelerating bone growth on titanium implants. **Y. Jo**, B. Choi, C. Kim, H.J. Cha

BIOT **307.** Design of experiments applications in bioprocessing: Chromatography process development. **L. Kanwar**, A. Godara, V. Kumar, A.S. Rathore

BIOT **308.** Optimization of titer and quality of IgG antibody using high-throughput micro-bioreactor system for CHO cell media, supplements and anti-foam screening. A. Williams, C. Hsu, **S. Velugula**, K.A. Brorson, C. Agarabi

BIOT **309.** Temporal and temperature-dependence on expression of Atrazine-degrading genes in *Pseudomonas* sp. ADP biofilms. **M.A. Delcau**, T.L. Peeples

BIOT **310.** Integration of HTPD and general interpolation models to predict overloaded chromatographic behavior. **A. Creasy**, G. Carta

BIOT **311.** Rational molecular tweaking of an IgG1 monoclonal antibody for improved high concentration solution properties. **K. Roffi**, S. Kumar

BIOT **312.** Biodegradation of sulfamethoxazole in sewage and swine sludge. C. Fan, **B. Chang**, L. Tsai

BIOT **313.** Engineering of microbial expression platform for antibodies fragments with scale-up process. **C. Fan**

BIOT **314.** Solvent stability and synthetic applications of an esterase isolated from moderately halophilic microrganism. **S. Toro**, **M. Abed**, J.J. Sanchez, A. Miranda, I. Rivera, **E. Fasoli**

BIOT **315.** Investigating C-terminal cleavage of amino acid residues in recombinant IgG produced in Chinese hamster ovary cells. **D. Ruble**, B.A. Kelly, B. Evans, P. Slade

BIOT **316.** Evaluating implications of high-temperature short time treatment on media component solubility and cell culture performance. **N. Moore**, E. Hodgman, C. Leung, J. Mullberg, E. Garr

BIOT **317.** Detection of small molecule via the application of VH and VL fragments of scFv: An example of bisphenol A sensing. **L. Yu-chun**, C. Chi, C. Chao, Y. Li, H. Ueda

BIOT **318.** Probing the lysine proximal microenvironments within membrane protein complexes by active dimethyl labeling and mass spectrometry. **Y. Wu**, Y. Zhou, F. Wang

BIOT **319.** High throughput screening under weak partitioning conditions to guide process development of monoclonal antibodies. **M. Aswath**

BIOT **320.** High-throughput combinatorial differentiation screening of 3D human neural progenitor cells for enhanced neurogenesis on a microarray chip platform. **G.J. Nierode**, B.C. Perea, S.K. McFarland, D.V. Schaffer, D.S. Clark, J.S. Dordick

BIOT **321.** Novel design of glutamine-derived polymer with a high affinity to cancer cells based on aberrant glutamine metabolism. **Y. Honda**, N. Yamada, H. Takemoto, T. Nomoto, M. Matsui, K. Tomoda, N. Nishiyama

BIOT **322.** In vitro – in vivo liver toxicity correlations of 3D microculture and humanized liver mice. **D. Bruckner**, M. Connerney, G. Monastersky, T. Little, J.S. Dordick

BIOT **323.** Molecular design of β-sheet-forming self-assembled peptides as common amyloid inhibitors. **R. Hu**, B. Ren, M. Zhang, H. Chen, J. Zheng

BIOT **324.** Process conditions that control cysteine/cystine associated product quality attributes. **J. Guthrie**, E. Yu, A. Saati, L. Wafer, P.G. Slade

BIOT **325.** Optimization of cell culture media to increase cell specific productivity and suppress cell growth in perfusion cell culture. **L. Zheng**, H. Lin, S. Wang

BIOT **326.** Self-assembled Iron Sulfide Supraparticles as Artificial Viruses. **E.S. Turali-Emre**, A.E. Emre, N. Kotov

BIOT **327.** Development of a two-step purification platform for *E. coli*-expressed Fab constructs. **W. Evans**, A. Chakrabarti

BIOT **328.** Engineering EF-Tu to translate unnatural amino acids with broader applications in synthetic polymer synthesis. **V. Cox**, E. Gaucher

BIOT **329.** Antimicrobial and anti-biofilm activities of extracted by supercritical fluid from *Moringa Oleifera* seed. **J. Park**, Y. Kwon, C. Kim, Y. Kim, J. Lee, G. Gwon, J. Lee

BIOT **330.** Developing a simple and versatile platform for pathogen detection utilizing engineered DNA-binding proteins. **S. Alam**, A. Brown, S. Chung, M. Chung, M. Kim

BIOT **331.** XDR-500 MO—single-use fermentor for microbial processes. J. Vasi, **A. Castan**, S. Kristiansson

BIOT **332.** Control of glycation and deamidation of monoclonal antibodies by high-throughput screening via ambr250 technology. **M. Moynihan**, N. DePrimo, P.J. Alfonso, J. Grey

BIOT **333.** Production of IL-24 and its receptors for structural studies. **C. Sonmez**, J. Lubkowski, A. Wlodawer

BIOT **334.** Probing hGFAT1 activity through small-molecule inhibition, CRISPR and Cryo-EM: Identifying the downstream effects of O-GlcNAc modified proteins and their role in cancer cell survival. **L.A. Walter**, Y. Lin, K.N. Chuh, F. Nasertorabi, R. Stevens, M. Pratt

BIOT **335.** Using metalloproteins as targets to develop antimicrobial agents. **Y. Chen**, Z. Zhang, H. An

BIOT **336.** Engineering polyketide synthases for production of designer biofuels. **A. Zargar**, R. Phelan, C.B. Bailey, L. Katz, J.D. Keasling

BIOT **337.** High throughput resin screening and development of polishing chromatography step for a recombinant therapeutic protein. **X. Pan**, Y. Chang, J. Teare, H. Tjandra, A. Hesslein

BIOT **338.** Designed coculture for the production of metabolites from air, water and sunlight. **M.J. Smith**, M.B. Francis

BIOT **339.** Long-term storage solution offering membrane stability and bioburden effectiveness for regenerated cellulose ultrafiltration membrane cassettes. **W. Cataldo**, D. Aquino, M. Kozlov, D. DeCesaro, K. Souza, A. Bartlett

BIOT **340.** Evaluating the correlation between packing quality and process performance in protein A chromatography. A. Becerra-Arteaga, **J. Castano**

BIOT **341.** Development and evaluation of synthetic 3D scaffolds for the maintenance of viability and function of hepatocytes. **J.A. Hoch Brown**, P. Das, L. Tan, J.A. Wertheim

BIOT **342.** Effects of pore size on protein binding capacity of affinity membranes. A. Santiago Ruiz, **C. Ortiz Hernandez**, R. Oyola Martinez, **E. Fasoli**, **V. Bansal**

BIOT **343.** Evaluation of the Virosart® media filter for application in upstream risk mitigation for adventitious agent contamination. R. Alsop, **C. Breuning**, H. Aranha

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

BIOT **344.** Using multimodal chromatography: Developing an effective and robust purification process for a bispecific antibody. **E. Rosenberg**, **S. Willmann**, S. Konrad, S. Hackl

BIOT **345.** Influenza virus capture using membrane chromatography: Improving selectivity by matrix design and pseudo-affinity ligand interactions. **H. Kaligotla**

BIOT **346.** Chinese Hamster Ovary (CHO) cell specific high throughput multiplex glycosylation assay. **S. Gupta**, C. Goudar, J. Piret

BIOT **347.** Modular approach of supramolecular complexation with chemically conjugated peptide building blocks. **E. Kang**, Y. Kim

BIOT **348.** Continuous chromatography for polishing of biomacromolecules: A reliable alternative to traditional batch chromatography? . **C. Wayne**, A. Velayudhan

BIOT **349.** Directed evolution of CRISPR/Cpf1 for orthogonal PAM recognition. **Z. Abil**, J. Gollihar, J. Ellefson, I. Finkelstein, A.D. Ellington

BIOT **350.** Facile affinity maturation of antibody variable domains via natural diversity mutagenesis. **K. Tiller**, T. Li, R. Chowdhury, C. Maranas, P.M. Tessier

BIOT **351.** Application and strategy of leveraging prior knowledge to facilitate process validation activities. **S. Wong**, K. Kaleas, M. Hutchinson, A. Kleinjans, A. White, J. Persson

BIOT **352.** Investigation of protein monomer-aggregate separations using multimodal chromatography. **L. Zhang**, J. Chen, S.M. Cramer

BIOT **353.** Improvement of gamma-aminobutyric acid production by an overexpression of glutamate decarboxylase from *Pyrococcus horikoshii* in *Escherichia coli*. **S. Hong**

BIOT **354.** Development of recA promoter based bisphenol-A sensing and adsorption system by recombinant Escherichia coli. **S. Hong**

BIOT **355.** Increased salinity tolerance: Linked with the sodium transporter HKT1. **R. Nadipalli**

BIOT **356.** Isoelectric chromatofocusing as an analogous technique to isoelectric capillary electrophoresis for preparation separation of monoclonal antibodies. **D. Choy**, S. Sen, X. Zhang, S. Voronov, N. Chittoor

BIOT **357.** Effect of matrix on protein separation and capacity with multimode ligands. **B. Thiyagarajan**, Q. Zhang, H. Li, B. Beyer, N. Deorkar

BIOT **358.** Identification and control of a unique glycosylation sensitivity in a bispecific immunoglobulin. **B. Shepard**, C. Racicot, K. Chemfe, L. Zhou, A. Ibraghimov, D. Serna, P. Hossler

BIOT **359.** Adapting single-use mixing solutions for high titer drug product formulation: A case study. **A. Sokolnicki**

BIOT **360.** Fluorescent precipitation-based sensing of nucleic acid targets using carbon-dot nanoparticles for detecting multidrug-resistant bacteria. **H. Lee**, J. Ryu, H. Chung

BIOT **361.** Graphene as a protective dental layer and an antimicrobial agent for the prevention of biofilm formation. **S. Grace**

BIOT **362.** Utilizing a step-wise approach to define binding mechanisms of virus particles to multimodal anion exchange resin. **M. Brown**, S. Johnson, K.A. Brorson, S. Lute, D.J. Roush, J. Hughes, M. Burnham, F. Wang, A. Walsh

BIOT **363.** Process economy modeling for viral vector production. **M. Bennemo**, G. Ahlén, T. Persson, Ä. Hagner Mcwhirter, M. Lundgren

BIOT **364.** Online biocapacitance probes for the monitoring of viable cell density and automating feeding strategies in mammalian cell cultures. **D. Monteil**, P. Cheng, H. Lin, D. Bock

BIOT **365.** Application of perfusion technology for improvement of a legacy biologics process. **D. Harrison**, N. Vaidyanathan, E. Garr

BIOT **366.** Directed evolution of an epoxide hydrolase: Engineering the active site of the Cif epoxidase to form a covalent bond with progressively larger synthetic substrates. **M. Ko**, J.J. Love

BIOT **367.** Evaluating the impact of high extracellular lactate on induced pluripotent stem cell metabolism and pluripotency. **D. Odenwelder**, S.W. Harcum

BIOT **368.** Withdrawn.

BIOT **369.** Should charge variants of monoclonal antibody therapeutics be considered critical quality attributes? . **D. Kumar**, S. Singh, G. Narula, A.S. Rathore

BIOT **370.** Risk mitigation for calcium chloride solution as an additive to cell culture media using high flux virus filters. **R. Alsop**, C. Breuning, H. Aranha

BIOT **371.** Novel approache to the chemical similarity networks that will improve the drug target identification. Y. Lo, **G. Ren**, E.J. Parish, **H. Honda**

BIOT **372.** Novel approaches to the wireless system on sensor networks with new device to agricultural environment. G. Ren, E.J. Parish, Y. Lo, **H. Honda, M. Hsiao**, T. Wei

BIOT **373.** Novel application of new bioinformatics methods to glycoprotein identification and functional prediction. **G. Ren**, E.J. Parish, Y. Lo, **H. Honda**

BIOT **374.** Novel application of scanning electron microscopes and the comparison of non-native tephritid flies. G. Ren, **H. Honda**, Y. Lo, E.J. Parish, T. Wei

BIOT **375.** Novel approaches to the clinical efficacy study of the application of ticagrelor for the PCI patients. **L. Lv**, D. Ren, E.J. Parish, G. Ren, **H. Honda**

BIOT **376.** Novel approaches to the development of amperometric biosensor for serum cholesterol level determination. Y. Lo, G. Ren, **H. Honda**, M. Hsiao, T. Wei

BIOT **377.** New approaches to the chemical synthesis of azetidinone, naturally occurring β-lactam antibiotics. **D. Ren**, Y. Lo, G. Ren, E.J. Parish, **H. Honda**

BIOT **378.** Engineering Bone Morphogenetic Protein-1 (BMP-1) in *Saccharomyces cerevisae* as a potential treatment of osteoarthritis. **R. Yaghi**, B. Iverson

BIOT **379.** Withdrawn.

BIOT **380.** Deciphering and expending *Clostridium formicoaceticum* metabolism based on whole genome sequencing. **T. Bao**, S.T. Yang

BIOT **381.** Single-Molecule and isocratic protein competition on ion-exchange adsorbents. **U. Patil**, L. Kisley, S.P. Dhamane, M. Poongavanam, A. Mansur, E. Kulla, L.J. Tauzin, K. Kourentzi, C.F. Landes, R.C. Willson

BIOT **382.** Novel approach for transdermal delivery of ferulic acid via microneedle. B. Zhong, H. Poon, W. Han, **M. Hasan**, K. Yeung

BIOT **383.** Sustained release of small molecules from silk films with applications in HIV-inhibition. **J. Andersen**, P.J. Liwang, L. Zhang

BIOT **384.** Ultrasound activated and fluorescent film for *in vivo* bio-imaging. **J. Yang**, E. Ward, T. Sung, J. Wang, C. Barback, N. Mendez, J. Delong, S. Blair, W.C. Trogler, A. Kummel

BIOT **385.** Identified genes involved in improving recombinant protein expression from HEK 293 cells by miRNA 22-3p. **S. Inwood**, M.J. Betenbaugh, J. Shiloach

BIOT **386.** Single-use bioreactor selection and scale-up considerations for live virus vaccine production. S. Christanti, **J.C. Gercke**, K. Hamaker, D. Jan

BIOT **387.** Controlling quality attributes in an Fc fusion protein through the manipulation of cell culture pCO2. **D. Maskas**, E. Garr

BIOT **388.** Preparation, crystallization, microstructure and mechanical behavior of silica based biocompatible glass ceramics for dental applications. **C. Gautam**

BIOT **389.** Supramolecular assembly of β-peptides nanofibers with carbon nanotubes formed by noncovalent helical wrapping. **J. Nam**, N. Kim, O. Lee, Y. Kim

BIOT **390.** Engineered conductive and biodegradable bio-ionic liquid hydrogel. **J. Pletcher**, **M. Isterfi**, M. Nabavinia, M. Keshvardoost, S. Asgari, A. Masoumi, I. Noshadi

BIOT **391.** Strategy for qualifying a mechanistic chromatography modeling approach. **C. Williams**

BIOT **392.** Hydrogen-deuterium exchange to interrogate the reaction kinetics of d-glucuronyl C5 epimerase. **D. Vaidyanathan**, L. Lin, K. St. Ange, X. Zhang, B. Cress, C. Wang, R.J. Linhardt, J.S. Dordick

BIOT **393.** Comprehensive characterization of the cellulosome machinery of three novel strains of anaerobic gut fungi. **D. Knop**, M.A. O'Malley

BIOT **394.** Evaluation of Flow-VPE for in-line concentration measurement of monoclonal antibodies during chromatography. **P. Shah**, M. Rohani, K. Mehta, B. Yao, R.G. Soderquist

BIOT **395.** Modeling and simulation in the biotech industry: A survey from the 2nd workshop. **J. Griesbach**, A. Staby, R.J. Todd, S. Hunt

BIOT **396.** Versatile signal peptide for periplasmic translocation of heterologous proteins in *Escherichia coli*. **J. Seo**

BIOT **397.** Development of polydiacetylene-phospholipid based biosensors for the detection of influenza virus and Foot and Mouth Disease Virus (FMDV). **J. Jeong**, T. Kim, I. Lee, S. Jung

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BIOT **398.** Mechanism of filter fouling of virus retentive membranes. **M. Bieberbach**, M. Bennecke, P. Kosiol

BIOT **399.** Characterizing anaerobic fungal sugar transporters for metabolic engineering applications. **I. Podolsky**, S. Seppala, M.A. O'Malley

BIOT **400.** Creating the ideal vaccine formulation: Attenuating inflammation while maininting the adaptive respsone. **B. Moser**, R.C. Steinhardt, B. McGonnigal, Y. Escalante-Buendia, A. Esser-Kahn

BIOT **401.** Developing polyvalent vaccines and therapeutics against viral pathogens. **T. Rosen**, C. Varner, A. Arsiwala, F. Krammer, R.S. Kane

BIOT **402.** Using metabolic flux analysis to analyze carbon flux in the C4, drought-tolerant crop sorghum. **S. Moore-Farrell**, C. Broeckling, A. Heuberger, C. Jahn, C.A. Peebles

BIOT **403.** Generation of high producing cell lines with suspension adapted DXB11-S1 in chemically defined medium and optimization of basal medium. **B. Chen**, H. Lu, W. Chi

BIOT **404.** Redirecting the immune response by controlling the nanoscale presentation of antigens. **C. Varner**, A. Arsiwala, T. Rosen, R.S. Kane

BIOT **405.** Insertion of inter-domain linkers improves expression and bioactivity of zygote arrest (Zar) fusion proteins. **J.M. Cook**, A. Charlesworth

BIOT **406.** Genetically encoded biotin analogs in bacterial and mammalian cells. **A. Hohl**, Y. Mideksa, M. Feige, K. Lang, J. Eppinger

BIOT **407.** Achieving ultra-high antibody concentrations. **P.J. Davis**

BIOT **408.** Facing the unknown: Suggesting alternative novel biochemistry in *Escherichia coli* and *Saccharomyces cerevisiae*. **A. Chiappino Pepe**, M. Ataman, N. Hadadi, H. Mohammadi, V. Hatzimanikatis

BIOT **409.** Manipulating sialylation of antibody fusion protein in cell culture process. **X. Chen**, L. Zhao, L. Fan, W. Tan

BIOT **410.** Using natural ligand and receptors to develop next-generation cancer therapeutics. **J.W. Kim**, C. Marquez, A. Sweet-Cordero, J.R. Cochran

BIOT **411.** Artificial intelligence in protein chromatography: Estimation of mechanistic model parameters. **G. Wang**, T. Briskot, T. Hahn, P. Baumann, J. Hubbuch

BIOT **412.** Effect of yeast hydrolysate on monoclonal antibody production and auality: A transcriptomic perspective. **W. Buggele**, M.R. Good, W. Ling

BIOT **413.** Optimization of solid support and ligand density to improved alkaline stability of protein A resin. **J.U. Hansson**, D. Jansson, B. Noren, I. Eklind, J. Vasic

BIOT **414.** Understanding the generation of monoclonal antibody charge heterogeneity in CHO cell cultures. **X. Zhang**, H. Tang, L. Zhao, L. Fan, W. Tan, **X. Liu**

BIOT **415.** Disposable microliter monolithic columns for PAT. **A. Podgornik**, T. Lukan, N. Yoshimoto, S. Yamamoto

BIOT **416.** Optimization of high capacity protein A chromatography step for a therapeutic monoclonal antibody. **Y. Chang**, R. Zolyomi, X. Pan, K. Shill, G. Prakash, H. Ly, H. Tjandra, A. Hesslein

BIOT **417.** Development of microchip CE system for single-strand conformation polymorphism analysis. **G. Shin**, G. Jung

BIOT **418.** Controlling variability in protein therapeutics by defining trace metal and carbohydrate composition in upstream process development. **B. Beyer**, J. Fura, L. Fortin,. Thiyagarajan, N. Deorkar

BIOT **419.** Microcarrier removal using gradient depth filters: Influenza vaccine case study. **A. Gupta**, S. Patel, L. Mullin, M. Higson, C. Gillespie

BIOT **420.** Continuous antibody capture with a scalable supported bed platform. **G. Platteau**, G. Ströhlein, M. Siwak, G. de los Reyes

BIOT **421.** Investigating the use of Polyethyleneimine (PEI) in combination with tangential flow filtration for the primary recovery of antibody fragments from *E. coli* fermentation using ultra scale-down techniques. **J. Newton**, M. Hussain, J. Vlahopoulou, Y. Zhou

BIOT **422.** *In vitro* oxidative folding of disulfide-containing protein using aromatic thiols and disulfides. **N. Zhang**, **W.J. Lees**

BIOT **423.** Withdrawn.

BIOT **424.** Why complicate, when simple things can make big differences to your process. J. Kanakaraj, C. K.N, S. Desan, **D. Baskar**, A. Bhatnagar, A. Goel

BIOT **425.** Development, scale-up and proof of concept of a live virus vaccine platform using single use technology in the clinical space. **K. Apgar**, R. Ducoat, B. Grau, B. Thomas, F. Torres

BIOT **426.** Integrating transcriptome analysis and data driven prognosis to decipher catabolite repression. K. Wu, M. Gao, A. Chandra, **Z. Shao**

BIOT **427.** Nano-scale reversible oligomerization of amyloidogenic peptides. **K. Yokoyama**, J. Battaglia, J. Ehret, J. Bekoe, M. Endo, A. Islam

BIOT **428.** Characterization and removal of a monoclonal antibody aggregate containing four light chains. **Z. Tan**, V. Ehamparanathan, Y. Song, W. Hui, R. Swanson, S. Traylor, N. Singh, D. Yu, M. Lu, A.T. Lewandowski, Z. Li

BIOT **429.** Peptide conformational change effect to a solvent diffusion rate in a sol-gel matrix. **K. Yokoyama**, R. Sah, J. Ban, E. Esquivel, R. Singh

BIOT **430.** Investigation of peptide conformation through energy relaxation dynamics of fluorophore interacting with amyloid beta peptide at nanoscale interface. **K. Yokoyama**, T. James, J. Imayeguahi, A. Olatunbosun

BIOT **431.** Fusing individual-based models with genome-scale metabolic networks - a novel approach for quantifying emergent microbial community spatiotemporal dynamics. **M. Ataman**, B. Borer, D. Or, V. Hatzimanikatis

BIOT **432.** Aptameric sensor for fluorescent analysis of specific nucleic acid sequence. **N. Kikuchi**

BIOT **433.** Effects of flow and seeding on the crystallisation of immunoglobulin G. **H. Yang**, J. Heng

BIOT **434.** High throughput survivin promoter assay for embryotoxicity and cancer drug screening. **X. Xin**

BIOT **435.** Designing robust virus filtration processes to maximize operational flexibility while achieving small virus removal. **B. Buesing**, T. Hongo-Hirasaki, M. Inouye, D. Strauss, A.H. Schwartz, N. Hirotomi, T. Miyabayashi

BIOT **436.** Impact of an iron contaminant and its removal during downstream processing. **M. McClure**, S. Freeman, R. McCoy, B. Dell, D. Leiske, A. Gillespie, L. Connell-Crowley

BIOT **437.** Cyanobacterial genome-scale carbon mapping models for genome-scale 13C-metabolic flux elucidation. **S. Gopalakrishnan**, C. Maranas

BIOT **438.** Discovery, characterization and applications of a novel extremozymes from the deep Red-Sea brine pools. S. Grötzinger, A.L. Akal, M. Vogler, R. Karan, **J. Eppinger**

BIOT **439.** Peptide-conjugated smart biopolymers for the purification of therapeutic proteins by affinity precipitation. **A. Mullerpatan**, E. Kane, D. Chandra, P. Karande, S.M. Cramer

BIOT **440.** Alteration of bacterial surface protein architectures for guided assembly of cell populations. **J. Terrell**, H. Dong, M.C. Small, D.A. Sarkes, J. Jahnke, M. Hurley, W.E. Bentley, D.N. Stratis-Cullum

BIOT **441.** Withdrawn.

BIOT **442.** Integrated continuous protein A capture chromatography: Lean development approach. **R. Rodrigues**, H. Thuer, L.W. Pampel, J. Shultz

BIOT **443.** Combined electrophoretic and light scattering approach to elucidate the molecular origin of reverse Hofmeister series effects on protein solutions. **R. Curtis**, M. Nuhu, A. Alfutimie, D. Kovacevic

BIOT **444.** Systematic development of direct photosynthetic succinate production from CO2. E.I. Lan, **C.T. Wei**

BIOT **445.** Analytical characterization and establishing comparability of IgG1-based monoclonal antibody. **N. Nupur**, N. Chhabra, R. Dash, A.S. Rathore

BIOT **446.** Production of formate from carbon monoxide-containing waste gas using homoacetogenic bacteria as whole cell biocatalyst. **H. Hwang**

BIOT **447.** Separation by intrinsic magnetic susceptibility differences in cells. **K. Park**, T. Testoff, J. Adams, M. Venere, M. Zborowski, J. Chalmers

BIOT **448.** Process optimization for high cell density cultivations in cell culture-based viral vaccine production. **Y. Wu**, X. Liu, L. Zhao, Q. Ye, W. Peng, W. Dai, K. Hu, W. Tan

BIOT **449.** Removal of organic acids from bio-oils by catalytic esterification. J. Li, T. An, X. Bao, **H. Liu**

BIOT **450.** Peptide array and SAMDI mass spectrometry for profiling protein activities in cell lysates. **H. Kuo**, T. DeLuca, W.M. Miller, M. Mrksich

BIOT **451.** Fundamental toolbox for protein A resin characterization and link to application efficiency. **O. Rammo**, P. Menstell, B. Edelmann, R. Skudas

BIOT **452.** Tuning high mannose glycan levels of therapeutic proteins via CHO cell culture media supplementation. **J. Wang**, X. Chen, C. Wang, L. Zhao, W. Tan, **L. Fan**

BIOT **453.** Case analysis of orthogonal, sterile antibody purification platform. **R. Skudas**, O. Rammo, P. Menstell

BIOT **454.** Combining Rh-catalyzed diazo-coupling and enzymatic reduction to efficiently synthesize enantioenriched 2-substituted succinate derivatives. **Y. Wang**, **M.J. Bartlett**, C. Denard, J.F. Hartwig, H. Zhao

BIOT **455.** Ion-Specificity on reponsive hydrophobic interaction chromatography. X. Sun, **X. Qian**

BIOT **456.** Rapid and reliable analytical RP HPLC for high-throughput insulin process development. **A. Stein**, A. Heinen-Kreuzig, A. Kiesewetter

BIOT **457.** Case Study: Expedited development of a cation exchange polishing step for therapeutic monoclonal antibody purification using a miniaturized high-throughput approach. X. Pan, D. Surendar, Y. Chang, R. Zolyomi, **H. Tjandra**, A. Hesslein

BIOT **458.** Tracking the delivery of silver to bacteria. **M.N. Pinto**, I. Chakraborty, W. Schultz-simonton, M. Rojas-Andrade, P. Mascharak

BIOT **459.** Accelerated generation of high-yielding monoclonal stable CHO cell lines using a ClonePix-based cell line development platform. **K. Agarwal**, M. Kachole, A. McKenzie, J.G. Smedley, A. Shukla, A. Hussain

BIOT **460.** Scalability of cell culture processes in single-use bioreactors using different CHO cells line variants. **N. Bubna**, C. Phillips, S.S. Mostafa, A. Shukla

BIOT **461.** Systems biology approaches to omics data analysis in complex diseases. **R. Hajjo**, C. Willis

BIOT **462.** High-throughput screening of hydrolytic enzyme activity via wireless antennas with embedded (bio)-logic. **N.F. Reuel**

BIOT **463.** Using co-dominant negative recA to enhance CRISPR/Cas9-mediated recombineering. **E. Moreb**, M. Lynch

BIOT **464.** Novel clinically-relevant nanoscale probes for optical cell labelling and tracking. **D. Jasim**, K. Kostarelos

BIOT **465.** Molecular mechanisms of ion transport in a soy protein-based solid ion conductor. **J. Liu**, Y. Jewel, X. Fu, Y. Wang, W. Zhong

BIOT **466.** Refractive Index as part of a feedback control scheme to better control tangential flow filtration operations. **Y. Lam**, M. Westoby

BIOT **467.** Cell-selective proteomic analysis of host-microbe interactions using Bioorthogonal Noncanonical Amino Acid Tagging (BONCAT). **S. Stone**, J. Shon, A. Khosravi, M. Sweredoski, A. Moradian, S. Hess, S. Mazmanian, D.A. Tirrell

BIOT **468.** Withdrawn.

BIOT **469.** Downstream processing development of *Nicotiana benthamiana* based recombinant butyrylcholinesterase. **S. Alkanaimsh**, J. Corbin, K. Karuppanan, M. Kailemia, C.B. Lebrilla, R. Rodriguez, S. Nandi, K. McDonald

BIOT **470.** Harnessing intranodal vaccination to probe changes in local and systemic immunity. **J.I. Andorko**, J. Gammon, C. Jewell

BIOT **471.** Process Analytical Technology (PAT) in continuous bioprocessing. **E. Btonjic-Sehic**

BIOT **472.** Reverse hairpin beacon based positive SERS assay for influenza virus detection. **K. Jisun**, E. Jang, S. Han, J. Kim, Y. Huh, S. Haam

BIOT **473.** Withdrawn.

BIOT **474.** Process economy improvements with in-line conditioning using ready-made stock solutions in a mAb case study. **M. Hall**, K. Busson, T. Bjorkman

BIOT **475.** Alpha helix stabilization for improving the subcutaneous bioavailability of a helical peptide. **L. Zhang**, T. Navaratna, G. Thurber

BIOT **476.** Enabling Hyper-productive™ processing: Advances in a novel modular supported bed chromatography platform. **M. Siwak**, A. Naresh, G. de los Reyes

BIOT **477.** Single-molecule investigation of tau protein solution-phase conformations using the anti-Brownian electrokinetic (ABEL) trap. **L. Manger**, A. Foote, S. Wood, M.R. Holden, M. Margittai, R.H. Goldsmith

BIOT **478.** Application of chlorine dioxide as a bactericide agent. **R. Moore**, B.G. Ooi

BIOT **479.** Solid-state hydrogen-deuterium exchange mass spectrometry (ssHDX-MS) analysis of therapeutic fragment antigen-binding (Fab) protein formulations. **K. Balakrishna Chandrababu**, L. Kumar, B. Walters, D. Chang, P. Nayak, A. Allmendinger, I.E. Zarraga, E.M. Topp

BIOT **480.** Computational Fluid Dynamics (CFD) modeling of axial and radial flow distribution and its impact on fouling in Hollow Fiber Tangential Flow (HFTFF) and Alternating Flow (HFATF) microfiltration in perfusion bioreactor. **F. Radoniqi**

BIOT **481.** Nano-interface peptide affinity for amyloidogenic peptides. **K. Yokoyama**, P.J. Shevlin, K. Brown, M. Abdelmalik, A. Olatunbosun

BIOT **482.** Probing the local electronic structure of dilute bioinorganic active sites using ultra-sensitive soft X-ray detectors. **C. Titus**, B.K. Alpert, M.L. Baker, H. Cho, E. Denison, W.B. Doriese, J.W. Fowler, K. Gaffney, B. Gao, J. Gard, G.C. Hilton, K.D. Irwin, Y.I. Joe, C. Kenney, J. Knight, T. Kroll, S. Lee, D. Li, M. Minitti, K. M. Morgan, R.A. Mori, D. Nordlund, G. O'Neil, H. Ogasawara, C. Reintsema, D. Schmidt, D. Sokaras, Y. Song, D.S. Swetz, J. Ullom, T. Weng, C. Williams, B.A. Young

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

BIOT **483.** Engineering self-cleaving intein affinity tags for biosep-arations using yeast surface display. **S.D. Stimple**, M.J. Coolbaugh, Y. Fan, J. Westfall, D.W. Wood

BIOT **484.** Late-phase process improvement: Methods to increase titer while maintaining product quality. **M. Bennett**

BIOT **485.** Translation initiation is controlled by RNA folding kinetics via a ribosome drafting mechanism. A. Espah Borujeni, A. Reis, **H. Salis**

BIOT **486.** Full factorial analyses via novel high-throughput microculture platform reveal numerous interactions among stimuli within adult hippocampal neural stem cell niche. **R. Muckom**, S.K. McFarland, B.C. Perea, A. Rosenbloom, M. Gentes, D.S. Clark, D.V. Schaffer

BIOT **487.** Kinetic modeling approach for media formulation optimization in mammalian CHO cell-cultures. **H. Bhatia**, S. Yoon

BIOT **488.** Systems engineering of N-glycans for the production of recombinant proteins in mammalian cells. T. Le, **C. Stach**, M. McCann, S. O'Brien, X. Chen, L. Zhao, M. Smanski, W. Hu

BIOT **489.** Overcoming the challenges of moving from hydrolysate-containing media to chemically defined media for a high cell density perfusion cell culture process. **R. Chelikani**, F.H. Bacon, H. Yuan

BIOT **490.** Precise engineering of regulated mammalian gene expression through core promoter choice. **C. Ede**, Y.Y. Chen, X. Chen, M. Lin

BIOT **491.** Functionalization of graphene by using protein engineering. **A. Tyagi**, I.H. Abidi, Z. Luo

BIOT **492.** Fabrication of S-Adenosyl Methionine (SAM) biosensor via engineered virus like particles. **N. Bhokisham**, Y. Liu, A. Brown, G.F. Payne, J.N. Culver, W.E. Bentley

BIOT **493.** Novel clone selection technique reveals heterogeneity among HEK293T cells engineered to produce therapeutic extracellular vesicles. **P. Amaya**, M. Phelps, T. Schmittgen, J. Chalmers

BIOT **494.** Inducing cell death in cancer cells by targeted cytochrome c delivery via transferrin-cytochrome c conjugate. **M. Saxena**, Y. Delgado, R.K. Sharma, S. Sharma, S. Ponce De Leon Guzman, A.D. Tinoco, K. Griebenow

BIOT **495.** Template assisted and continuous crystallisation: Control of polymorphs, protein crystallisation and bioseparation. H. Yang, **J. Heng**

BIOT **496.** Novel stereoselective alcohol dehydrogenases from red-sea brine pools. **A.L. Akal**, **S. Grötzinger**, J. Eppinger

BIOT **497.** Development of Streptomyces sp. FR-008 as a promising chassis. **Q. Liu**

BIOT **498.** Choosing the right protein A affinity chromatography column can improve the process performance. N. Yoshimoto, **S. Yamamoto**

BIOT **499.** Demonstration of a highly productive and scalable continuous chromatography approach. X. Gjoka, R. Gantier, **M. Schofield**

BIOT **500.** TFF Optimization for small molecule processing. **E. Peterson**

BIOT **501.** Mussel protein-based injectable porous microspheres for *in situ* cell delivery. **Y. Jo**, K. Min, D. Kim, B. Kim, D. Kim, H.J. Cha

BIOT **502.** Peptoid-based microsphere-coated slides have increased performance in ELISA microarray. **S.L. Servoss**, G. Perez, B. Colford

BIOT **503.** Predicting and understanding aggregation of antibody therapeutics at air-water interfaces. **I. Shieh**, D. Leiske, A. Patel

BIOT **504.** Exploiting yeast glucan microparticles for immune cells and tissue targeting. **I. Salon**, A. Bajgar, F. Stepanek

BIOT **505.** Molecular assay for rapid detection of nuclear factor Kappa B. **Z. Wang**

BIOT **506.** Isolation of live CTCs for downstream analysis using the MagSifterTM: Rare cell isolation device. **M.B. Kerby**, K. Ziv

BIOT **507.** Extraordinary urinary excretion of thin graphene oxide sheets following intravenous administration and short circulation in blood. **D. Jasim**, K. Kostarelos

BIOT **508.** Withdrawn.

BIOT **509.** Applications of high throughput screening in the process development for monoclonal antibody purification. **T. Zhou**, X. Fu, Z. Zhang, L. Wang, M. Jin, J. Bock

BIOT **510.** Rapid design of integrated, orthogonal downstream bioprocesses using characterization of process-related impurities and *in-silico* tools. **S. Timmick**, C. Goodwine, N. Vecchiarello, S.M. Cramer

BIOT **511.** Withdrawn.i

BIOT **512.** Case-Study of qualifying a mammalian working cell bank for use in manufacturing of a commercial biologic. **P. Apostolidis**, L. Zhou, N. Patil, P. Thompson, M. Boyer, H. Graham, R. Bates

BIOT **513.** Modulating biologic quality attributes by applying high-throughput technologies and advanced statistics for media and process optimization. **J. Tian**, C. Oliveira, S. Egan, Z. Tan, J. Chen, J. Lee, M.C. Borys, Z. Li

BIOT **514.** Molecular dynamics simulations of organomimetic cluster nanomolecules. **P. Rehak**, Y. Han, P. Kral

BIOT **515.** Phospho-proteomic and transcriptomic data for fungal cell-wall repair pathway reveal new functionality. **C. Chelius**, L. Ribeiro, J. Kumar, S. Lincoln, R. Srivastava, S. Harris, M. Marten

BIOT **516.** Metabolic modeling of a multicellular nitrogen fixing cyanobacterium. **J. Gardner**, N.R. Boyle

BIOT **517.** Factors impacting filterability during primary clarification of monoclonal antibodies. A.M. Senczuk, **J. Basha**, A. Lee, J. Salm

BIOT **518.** Process intensification benefits and PAT in continuous chromatography. **H. Blom**, B. Westerlund, A. Almlen, T. Bjorkman

BIOT **519.** Morphing the pepto-type: Translation of IgG-binding peptides into their peptoid analogues. **H. Reese**, S. Menegatti

BIOT **520.** Improving protein A performance using chromatographic clarification strategy. **A. Voloshin**, B. Cope, T. Hill, M. Murray, J. Peart, M. Richardson

BIOT **521.** Bringing down the cost of MAb purification with novel resin designs. **H.J. Johansson**, P. Gilbert

BIOT **522.** When DoE fails: Mechanistic modeling for chromatographic manufacturability. **T. Hahn**, T. Huuk, T. Beck, J. Hubbuch

BIOT **523.** Design of ligand and solid support for high capacity protein A resin. **D. Jansson**, J.U. Hansson, B. Noren, I. Eklind, J. Vasic

BIOT **524.** Harnessing the intramolecular electrons of enzymes: An alternative pathway to enzymatic fuel cells. **C. Ji**

BIOT **525.** Integrated product removal of terpenoids with direct adsorption and membrane-assisted extraction. **L. Janoschek**, L. Grozdev, S. Berensmeier

BIOT **526.** Preferential crystallization for the purification of highly similar polyphenols. **M. Silva**, B. Vieira, M. Ottens

BIOT **527.** High-throughput screen for compounds that block aberrant protein aggregation using a fluorescent bacterial display system. **J.J. Love**, M. Ko

BIOT **528.** Investigating hydrodynamics in expanded bed adsorption systems using multiphase computational fluid dynamics. **V. Koppejan**, G. Ferreira, D. Lin, H. Wang, M. Ottens

BIOT **529.** DOPA redox regulation strategy of mussel adhesion using plaque foot proteins. **M. Shin**, B. Yang, H.J. Cha

BIOT **530.** Withdrawn.

BIOT **531.** Synthesis and use of dendronized HIC supports for the recovery of proteins. M. Mata-Gómez, J.A. Valencia-Gallegos, M.A. Rito Palomares, **J. González-Valdez**

BIOT **532.** Study of alpha casein potential as anticancer drug and development of a nano-sized targeted drug delivery system. **V.C. Barcelo Bovea**, E.N. Saladini-Alvarado, L.J. Delinois, F.M. Joaquin, Y. Delgado, K. Griebenow

BIOT **533.** Withdrawn.

BIOT **534.** Chromatographic process development for complex biological feedstocks. **S. Pirrung**, M. D. Pons Royo, D. Parruca da Cruz, L.A. van der Wielen, R.F. van Beckhoven, M. Eppink, M. Ottens

BIOT **535.** Role of disulfide bonding in protein aggregation. **L.E. Hanzly**, J.R. Barone

BIOT **536.** Effect of ionomer rigidity on the complex formation with block-catiomer and RNAs. **K. Hayashi**, S. Fukushima, H. Takemoto, K. Osada, N. Nishiyama, K. Miyata, K. Kataoka

BIOT **537.** Prediction of subsequent centrifuge problems by analyzing clean-in-place data. **L. Xu**, J. Erickson

BIOT **538.** CFD of mixing of multi-phase flow in a bioreactor using population balance model. **L. Kanwar**, A.S. Rathore, J. Sarkar, V. Loomba

BIOT **539.** Focused library approach to discover discrete dipeptide bolaamphiphiles for siRNA delivery. **A. Eldredge**, M. Johnson, N.J. Oldenhuis, Z. Guan

BIOT **540.** Discretized multi-level elution trajectories for preparative chromatography. **A. Sellberg**, N. Andersson, A. Holmqvist, B. Nilsson

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BIOT **541.** Development of a high-throughput immunofluorescence assay platform using a DNA-encoded streptavidin library for the rapid evaluation of protein-catalyzed capture agents. **A. McCarthy**, J. Kim, R. Henning, A. Mishra, R. Ng, A. Museth, J. Heath, E. Winson, J. Oh, J.R. Heath

BIOT **542.** Biolayer Interferometry using Fortebio™ Octet® for monitoring antigenicity of ENVs to guide process development. **N. Oien**, L.S. Wolfe, J. Devaney, C. Cameron, B.C. Peacor, J.G. Smedley, A. Shukla

BIOT **543.** Strategies for increasing *Saccharomyces cerevisiae* tolerance to medium-chain fatty acids. **P.B. Botero Besada-Lombana**, N.A. Da Silva

BIOT **544.** Investigating protein throughput, vmax values and virus removal efficiency of the paper based mille-feuille filter. **S. Gustafsson**, A. Mihranyan

BIOT **545.** Withdrawn.

BIOT **546.** Economic benefits of membrane chromatography versus packed bed column purification of therapeutic proteins expressed in microbial and mammalian hosts. **M. Kumar**, M. Thukkaram, R. Mendhe, A.S. Rathore

BIOT **547.** Withdrawn.

BIOT **548.** Fluorescent turn-on probes for wash-free mRNA imaging via covalent site-specific enzymatic labeling. **E.C. Zhou**, S. Alexander, N.K. Devaraj

BIOT **549.** Colorimetric and fluorescence based Aptasensors for the determination of hepatitis B e antigen. **R. Huang**, **N. He**

BIOT **550.** Stress sensitivity toolkit with spectroscopic characterization for development of robust biologic drug products. **M.E. Krause**, J.M. Wasylyk, D. Fichana, A.S. Narang, S. Deshmukh, N. Chennamsetty, M.L. Adams, R.B. Gandhi

BIOT **551.** Domain based understanding of activity and thermal stability. S. Kang, **Y.J. Yoo**

BIOT **552.** Engineering the pH optimum of hyaluronidase for improved targeting of hyaluronan overexpressing pancreatic tumors. **J. Hennigan**, M. Lynch

BIOT **553.** Influence of the architecture of chromatographic media on protein adsorption. **S.H. Koshari**, Y. Liu, N.J. Wagner, A.M. Lenhoff

BIOT **554.** Lipid-polymer hybrid nanoparticles: Photoacoustic imaging applied to ovarian cancer diagnosis. **C. Chen**, J. Jokerst

BIOT **555.** Optimization of structure of an aptamer discovered utilizing Ligand Guided Selection (LIGS) yields high affinity aptamer. **H.E. Zumrut**, S. Batool, N. Van, P. Mallikaratchy

BIOT **556.** Bioconversion of butanal and 13C acetaldehyde conversion in three strains of yeast. **N.O. Flynn**, J. Alvarez

BIOT **557.** Transcriptome analysis in high-producing CHO cell cultures: Strategies to design high-performing cell culture media. **A. Castan**, D. Reinhart, R. Kunert

BIOT **558.** Investigating correlation between biolayer interferometry and biological assay for potency assessment of biotherapeutics. **D. Kumar**, S. Singh, A.S. Rathore

BIOT **559.** Quality by Design (QbD) based process development for production of ranibizumab in *E. coli*. **D. Kumar**, J. Batra, J. Gomes, A.S. Rathore

BIOT **560.** Setting new standards for cleaning and sanitization of Protein A chromatography resins. **M. Wetterhall**, S. Musunuri, A. Ljunglöf, T. Bjorkman, E. Monie, A. Mattsson, A. Grönberg

BIOT **561.** Biological self-assembly for modularly modifying hepatitis B virus-like particles for cancer detection and treatment. **E. Hartzell**, H. Kim, W. Chen

BIOT **562.** Evaluation of ligand design for downstream processes: Impacts of ligand structure on ion-exchange membrane performance. **J.K. Rasmussen**, C.A. Bothof, S. Colak Atan, G. Griesgraber, R.T. Fitzsimons, F. Sgolastra, A.W. Vail

BIOT **563.** Withdrawn.

BIOT **564.** Achieving desired product quality for a CHO-derived monoclonal antibody. **J. Lakkyreddy**, M. Gawlitzek

BIOT **565.** Molecular insight on the inhibition of rate limiting step of cholesterol synthesis: Comparison of binding efficiency of statins – a platform for the screening of novel molecules. R. Jain, U. Agarwal, **S. Ayothiraman**, T. Panda

BIOT **566.** Optimization and integration of single-pass, continuous final formulation technologies for mAb purification. **B. Trafton**, J. Marshall, E. Ayturk

BIOT **567.** Investigation into Host Cell Protein (HCP) - Monoclonal Antibody (mAb) interactions In downstream bioprocessing. **S. Ranjan**, W. Chung, J.S. Bee, R. Hofele, J. HeidbrinkThompson, M. Zhu, D. Robbins, S.M. Cramer

BIOT **568.** Rapid fractionation of monoclonal antibody oxidation variants using laterally-fed membrane chromatography. **R.H. Sadavarte**, P. Madadkar, C. Filipe, R. Ghosh

BIOT **569.** Effect of hydrophobicity on the ultrasound contrast of silica nanoparticles. **F. Chen**, J.V. Jokerst

BIOT **570.** Automated and miniturized ProteinA affinity resin lifetime optimization studies. M. Geiss, C. Atzkern, **S.A. Oelmeier**, D. Boeth

BIOT **571.** Interactions in L-arginine solutions detected by proxy via relaxation dispersion NMR Spectroscopy of H/D Exchange at the ε-NH. **G. Khirich**, A. Nandy, J.C. Lin

BIOT **572.** Withdrawn.

BIOT **573.** Withdrawn.

BIOT **574.** Maximizing the functional lifetime of Protein A resins. **J.Y. Zhang**, S. Ghose, R.S. Gronke, S. Siva

BIOT **575.** Coenzyme engineering of NADP-dependent hyperthermophilic dehydrogenases toward small-size biomimetic coenzymes. **R. Huang**, Y. Zhang

BIOT **576.** Domain insertion of a beta roll-forming peptide into a thermostable alcohol dehydrogenase gives rise to calcium-dependent cofactor specificity. **W. Abdallah**, K. Solanki, S. Banta

BIOT **577.** Monitoring endogenous microRNA during adipogenesis via exocytosis-mediated signal secretion of liposomal probes. **S. Han**, B. Kang, E. Jang, J. Ki, M. Shin, H. Son, Y. Huh, S. Haam

BIOT **578.** pDADMAC flocculation & clarification of CHO cell culture harvest. **A. Gupta**, J. Castano, K.M. Pizzelli, S. Ryan

BIOT **579.** Advective flow membrane chromatography: Utilization of flow-through mode for scalable, single-use downstream mAb processing. **R. Overbeck**, X. Chen, M. Lin

BIOT **580.** HP-β-cyclodextrin as an inhibitor of amyloid-β aggregation and toxicity. **B. Ren**, R. Hu, M. Zhang, H. Chen, F. Yang, K. Chu, J. Zheng

BIOT **581.** Laser scanning confocal microscope as a tool for ligand density and protein binding estimation in affinity membranes. **J. Cruz-Lebron**, S. Yeldell, J. Sotero, V. Bansal, I. Dmoschowski, **E. Fasoli**

Section B

InterContinental San Francisco

Grand Ballroom B/C

Alan S. Michaels Award in the Recovery of Biological Products

M. A. O'Malley, T. M. Przybycien, V. Roy, *Organizers*, *Presiding*

5:00 BIOT **582.** Industrial perspective on applied science & engineering for biopharmaceutical process development. **B.D. Kelley**

WEDNESDAY MORNING

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Systems Biology & Omics Applications

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

H. Le, N. E. Lewis, *Presiding*

8:30 BIOT **583.** Assessing stability, chromatin accessibility and transcriptional activity of the Chinese hamster ovary cell genome. **A. Bandyoapdhyay**, Z. Lee, C. O'Brien, M. McCann, S. O'Brien, W. Hu

8:50 BIOT **584.** Lessons from the hamster: A combined omics approach to analyze CHO cell lines and *Cricetulus griseus* tissues. **K.M. Heffner**, M.J. Betenbaugh, D. BaycinHizal

9:10 BIOT **585.** Insights into the protein secretory pathway in filamentous fungi using random and targeted mutational approaches. **K. Boppidi**, L. Ribeiro, N. Rogers, A. Ramsey, S. Nelson, S. Lincoln, R. Srivastava, S. Harris, M. Marten

9:30 BIOT **586.** Proteomic and transcriptomic analysis reveals major metabolic shifts in cyanobacteria exposed to dynamic light environments. S. Park, B. Andersson, C. Shen, G. Peers, D.S. Dandy, **K.F. Reardon**

9:50 Intermission.

10:10 BIOT **587.** Metabolic flux rewiring and physiology in *E. coli* knockout strains. **M.R. Antoniewicz**

10:30 BIOT **588.** Development of a core model of CHO cell metabolism. **A. Richelle**, N.E. Lewis

10:50 BIOT **589.** Kinetic modeling of metabolism in clostridia. **S. Dash**, A. Khodayari, G. Stephanopoulos, L.R. Lynd, C. Maranas

11:10 BIOT **590.** On the shift-up to high lactate production in fed-batch culture of mammalian cells. **T. Le**, C. O'Brien, T. Phan, E. Liu, W. Hu

Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Vaccines, Gene Therapy Vectors, Cell Therapy, Stem Cell & Non-Protein Biological Products

M. Bakhshayeshi, R. Barros, V. Natarajan, A. Noyes, N. Tugcu, *Organizers*

M. Bakhshayeshi, A. Jungbauer, A. Noyes, *Presiding*

8:30 BIOT **591.** Challenges and advances in live virus vaccine process development. **M. Wenger**, A. Kristopeit, S. Christanti, J. Konietzko, J. Ma, K. Phillips, J. Vlasak, S. Wang, M. Woodling, J.G. Joyce

8:50 BIOT **592.** Recombinant prokaryotic lectins for affinity capture of HIV envelope proteins. **U. Bhaskar**, S.S. Mostafa, A. Shukla

9:10 BIOT **593.** Manufacturing process development challenges for exosomes, a new therapeutic platform for the delivery of biomolecules. **A. Noyes**, R. Bourdeau, K. Konstantinov, M. Mercaldi

9:30 BIOT **594.** Can oligonucleotide purification processes be improved to meet (or beat) future industry demands. **R.S. Gronke**, R. Joshi, K. Ruanjaikaen, Y. Fillon, H. Nguyen, F. Antia

9:50 Intermission.

10:10 BIOT **595.** Addressing the downstream challenges of viral therapy for cancer treatment – a study of rhabdoviral vector purification. **S. Shoaebargh**, M.F. Medina, A. Smith, J. Bell, B. Lichty, D.R. Latulippe

10:30 BIOT **596.** High resolution separation of virus-like particles and extracellular particles by convective media. P. Steppert, N. Lendero, T. Schneider, P. Aguilar, A. Tover, **A. Jungbauer**

10:50 BIOT **597.** Enabling technologies for efficient downstream processing of AAV viral vectors. **P. Hermans**

11:10 BIOT **598.** Virus safety for vaccines, viral vectors, and cell based therapies. **D. Asher**, A. Boumlic, P. Pattnaik, M. Wisher

Section C

InterContinental San Francisco

Union Square

Biophysical & Biomolecular Processes

Protein Conjugates & Materials

S. Alavattam, J. Moore, J. A. Van Deventer, *Organizers*

S. Alavattam, G. Thurber, *Presiding*

8:30 BIOT **599.** Modular design and functionalization of enzymatic hydrogels using a self-assembling protein building block. **S. Lim**, D.J. Glover, D.S. Clark

8:50 BIOT **600.** Understanding water interactions at the biomolecule/surface interface through neutron reflectometry. **W. Fies**, L.J. Webb

9:10 BIOT **601.** Microenvironment effect rather than proximity channeling causes the activity enhancement in enzyme cascade. **Y. Zhang**, H. Hess

9:30 BIOT **602.** Ultra-Sensitive protein detection with nanoparticle-proximity ligation assay. **H. Chen**, M. Crum, H. Goux, D. Chavan, B. Vu, K. Kourentzi, R.C. Willson

9:50 Intermission.

10:10 BIOT **603.** *In vivo* site-specific protein tagging with diverse amines using an engineered sortase variant. **J. Glasgow**, M.L. Salit, J.R. Cochran

10:30 BIOT **604.** Design of double-click stabilized p53-like peptides with serum-independent on-target efficacy. **L. Atangcho**, E. Khera, G. Thurber

10:50 BIOT **605.** Engineering complete in vivo synthesis of acylated proteins. **R. Menacho Melgar**, M. Lynch

11:10 BIOT **606.** Engineered polyelectrolyte multilayers to promote immune tolerance. **L.H. Tostanoski**, M. Guo, W. Royal, C. Jewell

Section D

InterContinental San Francisco

Telegraph Hill

Drug Product & Delivery

Devices & Biopharmaceutical Drug Delivery: Interactions & Strategies

T. Randolph, E. Sahin, *Organizers*

D. Doughty, C. Weikart, *Presiding*

8:30 BIOT **607.** Enabling patient centric drug products through innovation in devices and drug delivery. **A. Subramony**

9:10 BIOT **608.** Container-formulation interactions: A comparison of borosilicate glass vials and cyclic olefin polymer vials with novel silica-coated surfaces. **C.F. Chisholm**, J. Berggren, C. Weikart, T. Randolph

9:30 BIOT **609.** Withdrawn.

9:50 Intermission.

10:10 BIOT **610.** Paradigm shift: How a novel drug delivery technology can save formulation time and effort. **M. Huddleston**

10:30 BIOT **611.** Withdrawn.

10:50 BIOT **612.** Cellular migration, survival and gene expression on patterned collagen fibers. **M. Paukshto**

11:10 Panel Discussion.

Section E

InterContinental San Francisco

InterContinental B

Quality by Design

Case Studies on Product Understanding & Determination of Quality Attribute Criticality (CQAs)

J. Glassey, R. Godavarti, *Organizers*

M. Albarghouthi, P. Dalby, *Presiding*

8:30 BIOT **613.** Perspectives on the impact of quality by design (after a decade in the making!). **B.D. Kelley**

9:10 BIOT **614.** How to uncover critical quality attributes – Lessons learned applying CQA assessment tools to biologics. **N. Alt**, T.Y. Zhang, P. Motchnik, V. Quarmby, T. Schlothauer, H. Beck, T. Emrich, R. Harris

9:30 BIOT **615.** Balancing act: Leveraging literature and in-house characterization in CQA assessment. **R. Hofele**, W. Xu, J. Ahn, J. Wang

9:50 Intermission.

10:10 BIOT **616.** Identification of critical quality attributes of biotherapeutics: GCSF as a case study. **S. Singh**, D. Kumar, D. Yadav, A.S. Rathore

10:30 BIOT **617.** Strategies to streamline risk ranking and filtering in quality by design process validation. **M.P. Lee**, J.A. Patch, J. Persson, C. Williams, S. Wong

10:50 BIOT **618.** Exploiting mAb structure characteristics for rapid screening and a directed QbD implementation in process development. **J. Glassey**, M. Karlberg, A. Kizhedath, M. von Stosch, S. Wilkinson

11:10 BIOT **619.** Development of an integrated risk assessment strategy for process related impurities for biopharmaceutical production. **Y. Li**, H. Luo, S. Nicholson

Section F

InterContinental San Francisco

Sutter

Emerging Technologies

Stem Cells & Regenerative Medicine

Y. Y. Chen, Y. Kim, J. P. Pieracci, *Organizers*

P. Apostolidis, S. Rao, *Organizers*, *Presiding*

8:30 BIOT **620.** Engineered tissue microspheres for use in regenerative medicine and disease modeling applications. **E.A. Lipke**

9:10 BIOT **621.** Metabolic transition between stem cell state and hepatocyte-like state. **D. Chau**, T. Le, Y. Park, W. Hu

9:30 BIOT **622.** High-throughput toxicity and phenotypic screening of 3D human neural progenitor cells on a microarray chip platform. **G.J. Nierode**, B.C. Perea, S.K. McFarland, D.V. Schaffer, D.S. Clark, J.S. Dordick

9:50 Intermission.

10:10 BIOT **623.** Megakaryocytic microparticles for cell-therapy applications: *In vitro* & *in vivo* studies. C. Kao, C. Escobar, **E.T. Papoutsakis**

10:30 BIOT **624.** Novel culture systems for trabecular meshwork and Schlemm's canal cells: An *in vitro* model for screening glaucoma therapeutics. **S.T. Sharfstein**, K. Torrejon, C. Dautriche, Y. Xie, M. Bergkvist, J. Danias

10:50 BIOT **625.** Engineering mechanical cues in the stem cell differentiation niche: Applications in vascular tissue engineering. **Q. Smith**, X. Yi Chan, A. Carmo, D. Vig, S. Sun, S. Gerecht

11:10 BIOT **626.** Fluid shear stress induces cancer stem cell-like phenotype in MCF7 breast cancer cell line without inducing epithelial-to-mesenchymal transition. **U.L. Triantafillu**, N. Klaassen, A. Raddatz, Y. Kim

Section G

InterContinental San Francisco

Grand Ballroom B/C

2017 E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in honor of Eleftherios T. Papoutsakis

Cosponsored by I&EC

M. A. O'Malley, T. M. Przybycien, V. Roy, *Organizers*, *Presiding*

11:30 BIOT **627. Award Address** (E. V. Murphree Award in Industrial & Engineering Chemistry sponsored by ExxonMobil Research & Engineering Company). 101 Years of clostridial biotechnologies. E.T. Papoutsakis

WEDNESDAY AFTERNOON

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Automated Technologies & High-Throughput Systems in Biologics

N. Agarwal, A. E. Schmelzer, I. R. Wheeldon, I. Yuk, *Organizers*

M. Jewett, A. Schmelzer, *Presiding*

2:00 BIOT **628.** Cell line development, miniaturization, automation, and analysis using the Berkeley Lights Platform. **K. Lee**, T. Neville, T.P. Munro

2:20 BIOT **629.** Shaken tube system for CHO process development. **P. Harms**, L. Chirdon, M. Gawlitzek

2:40 BIOT **630.** High-throughput scale down model (SDM) for fed-batch and perfusion process characterization studies. **S. Rameez**, J.S. Notey, D. Costello, D. Ryan, S.S. Mostafa, A. Shukla

3:00 BIOT **631.** Advancing automated sampling, process monitoring, and nutrient feedback control for a system of 3-L bioreactors. **K. O'Neill**, L. Hoshan, T. Seamans

3:20 Intermission.

3:40 BIOT **632.** Implementing HIPDOG (High end pH controlled delivery of glucose) in the AMBR15 microbioreactor system. **P. Jones**, B. Figueroa

4:00 BIOT **633.** Development of a CHO-based cell-free platform for the synthesis of active monoclonal antibodies as a potential high-throughput screening tool. **R. Martin**, N. Majewska, C. Chen, A.E. Schmelzer, M.C. Jewett, V. Roy

4:20 BIOT **634.** High-Throughput characterization of enzymes that assemble glycoproteins. **M. Mrksich**, M.C. Jewett, W. Kightlinger, L. Lin

4:40 BIOT **635.** Real time product quality analysis of mammalian cell culture processes. **M. George**, G. Sidhu, A. Durve, G. Sharma, J. Tressel, H. Lin, E. Zimmermann

Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Technology Transfer, Scale-Up & Scale-Down

R. Barros, V. Natarajan, N. Tugcu, *Organizers*

B. Roman, S. A. Tobler, *Presiding*

2:00 BIOT **636.** Use of platform strategy to achieve efficient and agile technology transfer. **M. Ratna**

2:20 BIOT **637.** Defining a window of operation by applying integrated fermentation and cell removal scale-down mimics of mammalian cell culture with predictive modelling. **M. Sebastian**, S. Goldrick, A. Mason, D. Gruber, R. Turner, S. Farid

2:40 BIOT **638.** Evaluation of single use harvest technologies. **A. Brinkmann**

3:00 BIOT **639.** Does BPOG extractable protocol truly help? - Case studies from an end user perspective. **E. Mahajan**

3:20 Intermission.

3:40 BIOT **640.** Optimization and scale-up of charge variants separation of mAbs in cation exchange chromatography. F. Wittkopp, F. Seelinger, **C. Dr. Frech**

4:00 BIOT **641.** Mechanistic investigations of chromatography resin aging: Building a toolbox to maximize the lifetime of resins used in commercial processes. **A.J. Pike**, P.R. Smith, B.F. Marques, K.E. Goklen

4:20 BIOT **642.** Scale-up and predicting flux-pressure relationships of Tangential Flow Filtration (TFF) using a combined Computational Fluid Dynamics (CFD) and Ultra Scale-Down (USD) input: Method and application. **M. Hussain**, Y. Zhou

4:40 BIOT **643.** Scalable and representative: Improved approaches to process characterization for a tangential-flow ultrafiltration unit operation. **A. Szkodny**, J. Molek, K.E. Goklen

Section C

InterContinental San Francisco

Union Square

Drug Product & Delivery

Big Data & Biomanufacturing

T. Randolph, E. Sahin, *Organizers*

J. Fox, A. Vatsyayan, *Presiding*

2:00 BIOT **644.** Learning from small data in the era of big data for real-time biopharmaceutical process monitoring. **A. Tulsyan**, C. Garvin, C. Undey

2:20 BIOT **645.** Application of multivariate data analysis to enhance product quality of a novel antibody-peptide fusion. **S. Goldrick**, W. Holmes, N. Bond, M. Kuiper, R. Turner, S. Farid

2:40 BIOT **646.** High-throughput data analysis for rapid ranking of high-concentration monoclonal antibody formulations using manufacturability indices. **Y. Yang**, A. Velayudhan, S. Farid, N. Thornhill

3:00 BIOT **647.** Fermentanomics: Relating quality attributes of a monoclonal antibody to cell culture process variables and raw materials using multivariate data analysis. **S. Singh**, M. Pathak, E. Read, C. Agarabi, A.S. Rathore

3:20 Intermission.

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

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3:40 BIOT **648.** Multi-objective medium-term capacity planning for stainless steel and single-use multi-product biopharmaceutical facilities under uncertainty using a genetic algorithm. **K. Jankauskas**, A.P. Long, M.D. Osborne, G.R. McCartney, L. Papageorgiou, S. Farid

4:00 BIOT **649.** Multivariate data analysis for biotech processes: Industrial case studies. **A.S. Rathore**, S. Singh

4:20 Panel discussion.

Section D

InterContinental San Francisco

Telegraph Hill

Bio-Based Products

Synthetic Biology Tool Development & Metabolic Engineering in Novel Microbes

M. R. Antoniewicz, C. A. Eckert, G. Sriram, *Organizers*

G. Rudenko, F. Zhang, *Presiding*

2:00 BIOT **650.** Pathway engineering pipeline for efficiently engineering many-enzyme pathways. S. Halper, D. Cetnar, **H. Salis**

2:20 BIOT **651.** Synthetic biology tools for engineering members of the marine bacterial genus *Vibrio*. **T. Tschirhart**, Z. Wang, J. Erickson, J. van Kessel, G.J. Vora

2:40 BIOT **652.** Light-dark cycle tool development in *Synechocystis sp*. PCC 6803. **A.J. Zimont**, D. Miller, C.A. Peebles

3:00 BIOT **653.** Synthetic biology tools for engineering *Gluconacetobacter sp*. **S. Lim**

3:20 Intermission.

3:40 BIOT **654.** Metabolic analysis of the extremely thermoacidophilic sulfolobales offers improved understanding of lithoautotrophy and identifies potential routes to production of bio-based chemicals and fuels directly from CO2. **B. Zeldes**, A. Loder, C. Straub, R. Kelly

4:00 BIOT **655.** Production of industrial products from natural gas using an engineered methanotroph biocatalyst. J. Kealey, **L. Chao**

4:20 BIOT **656.** Withdrawn.

4:40 BIOT **657.** Overcoming the transformation hurdle of *Clostridium cellulovorans* for efficient metabolic engineering towards consolidated n-butanol production from cellulose. **J. Zhao**, S.T. Yang

Section E

InterContinental San Francisco

Sutter

Emerging Technologies

Stem Cells & Regenerative Medicine

Y. Y. Chen, Y. Kim, J. P. Pieracci, *Organizers*

P. Apostolidis, S. Rao, *Organizers*, *Presiding*

2:00 BIOT **658.** Vocal fold-mimetic environment for the modulation of stem cell behaviors. **X. Jia**

2:20 BIOT **659.** Engineered environments for modulating iPSC function and fate in three-dimensional culture. **E. Ovadia**, A.M. Kloxin

2:40 BIOT **660.** Increasing stem cells retention and survivability by engineering with magnetic porous nanoparticles. **F. Chen**, E.R. Zhao, S. Darmadi, J.V. Jokerst

3:00 BIOT **661.** Scalable production of self-aggregating glioblastoma cancer stem cells. **J. Park**, Y. Kim

3:20 Intermission.

3:40 BIOT **662.** Solutions for robust cell therapy production. A. Schnitzler, M. Pease, T. Hood, T. Lawson, S. Luther, A. Verma, S. Punreddy, S. Rigby, **J. Murrell**

4:00 BIOT **663.** Reflectin as a material for neural stem cell growth. **R. Kautz**, L. Phan, J. Arulmoli, J. Kerr, M. Shenk, M. Pathak, L. Flanagan, F. Tombola, A.A. Gorodetsky

4:20 BIOT **664.** Functionalized poly(ethylene glycol)-based hydrogels as a synthetic culture surface to enhance in-vitro proplatelet formation. **E.N. Bess**, J. Berry, W.M. Miller

4:40 BIOT **665.** Amplified photodegradation of cell-laden hydrogels through an addition-fragmentation reaction. **T. Brown**, I. Marozas, K.S. Anseth

WEDNESDAY EVENING

Section B

InterContinental San Francisco

Grand Ballroom B/C

D.I.C. Wang Award Lecture

M. A. O'Malley, T. M. Przybycien, V. Roy, *Organizers*, *Presiding*

5:00 BIOT **666.** Following the advice of Daniel Wang: Improving quality through cell culture engineering. **M.J. Betenbaugh**

THURSDAY MORNING

Section A

InterContinental San Francisco

Grand Ballroom A

Upstream Processes

Engineering Natural Products Biosynthesis

N. Agarwal, I. R. Wheeldon, I. Yuk, *Organizers*

Y. Li, J. Wee, *Presiding*

8:30 BIOT **667.** Heterologous microbial (combinatorial) biosynthesis of natural products using dynamic metabolic control. **Z. Ye**, M. Lynch

8:50 BIOT **668.** Engineered biosynthesis of the complex natural products erythromycin and yersiniabactin for health and environmental opportunities. **B.A. Pfeifer**

9:10 BIOT **669.** Snake antivenom peptide production using elastin-like peptide tag. **C.F. Komives**, E. Hartzell, E.E. Sanchez, M. Suntravat, S. Mancini, W. Estell, K. Kumar, W. Chen

9:30 BIOT **670.** Design of synthetic microbial communities for metabolic engineering and synthetic biology applications. **J.A. Jones**, M. Koffas

9:50 Intermission.

10:10 BIOT **671.** Engineered biosynthesis of neoantimycin depsipeptides in S. albus J1074. **W. Skyrud**, J. Liu, W. Zhang

10:30 BIOT **672.** Design and implementation of a robust *S. cerevisiae* chassis strain with improved growth characteristics and stationary phase glycolytic flux. **J. Burg**, M. Lynch

10:50 BIOT **673.** Expressing a metabolic loop enables the continuous synthesis of 3-hydroxybutyrate in cyanobacteria. **T.T. Ku**, E.I. Lan

11:10 BIOT **674.** Metabolic engineering of *Synechocystis sp*. PCC 6803 for improved terpenoid production: Ribosome binding sites and codon optimization. **J. Sebesta**, C.A. Peebles

Section B

InterContinental San Francisco

InterContinental C

Downstream Processes

Advances in Non-Chromatographic Separations

R. Barros, V. Natarajan, N. Tugcu, *Organizers*

A. Azevedo, E. Benabaji, *Presiding*

8:30 BIOT **675.** Effect of channel induced shear on biologics during ultrafiltration/diafiltration. **A. Arunkumar**, N. Singh, M. Peck, E. Schutsky

8:50 BIOT **676.** Mechanisms of precipitation on pH adjustment. D.G. Greene, L. Choe, S. Traylor, N. Singh, X. Xu, Z. Li, K. Lee, N.J. Wagner, **A.M. Lenhoff**

9:10 BIOT **677.** Protein precipitation via combined reversible cross-linking and volume exclusion: Solubility and aggregation kinetics models. **T.M. Przybycien**, Q. Gu

9:30 BIOT **678.** Antibody aggregate removal by depth filtration in cell culture harvesting. **D. Yu**, M. Mayani, Y. Song, Z. Xing, Z. Li

9:50 Intermission.

10:10 BIOT **679.** Transitioning from low to high density mammalian cell culture clarification within existing manufacturing infrastructure. J. Walker, A. Richardson, **M. Westoby**

10:30 BIOT **680.** Effect of product concentration on continuous parvovirus-retentive filtration. **D. Bohonak**, H. Lutz

10:50 BIOT **681.** Investigation of flushing strategies for reducing beta glucan leachables originating from cellulose based depth filtration media. **A. Gupta**, D. Kinzlmaier, K.M. Pizzelli, E.M. Goodrich

11:10 BIOT **682.** Characterizing protein concentration dependent parvovirus filtration fouling. **A. Seay**

Section C

InterContinental San Francisco

InterContinental B

Drug Product & Delivery

Biopharmaceuticals: Novel Formulations & Mechanisms

M. E. Krause, T. Randolph, E. Sahin, *Organizers*

B. Demirdirek, *Organizer, Presiding*

M. Krause, *Presiding*

8:30 BIOT **683.** Melt processed virus-like particle laden polymeric implants for immunoresponsive applications. **P. Lee**, S. Shulka, J.D. Wallat, C. Danda, J. Maia, N. Steinmetz, J.K. Pokorski

8:50 BIOT **684.** 2-Nitrobenzenesulfonamide group as a chemical linker with highly selective cleavability in response to intracellular redox system for a construction of siRNA-polymer conjugate. **H. Takemoto**, C. Huang, T. Nomoto, K. Tomoda, M. Matsui, N. Nishiyama

9:10 BIOT **685.** Peptide dendrons as thermal stability amplifiers for IgG1 monoclonal antibody biotherapeutics. **R. Bansal**, S. Chattopadhyay, A.S. Rathore, S. Dhawan, V. Haridas

9:30 BIOT **686.** Aptamer-peptide-drug conjugates: Targeted delivery of synergistic drug combinations with ratiometric precision. **A. Pusuluri**, S. Menegatti, H. Soh, S. Mitragotri

9:50 Intermission.

10:10 BIOT **687.** Withdrawn.

10:30 BIOT **688.** *In vitro* selection of pH-activated DNA nanostructures. **F. Fong**, S. Oh, C.J. Hawker, H. Soh

10:50 BIOT **689.** Brain targeting transferrin conjugated deformable nanovesicle (Tf-DNV) encapsulating the bioflavonoid galangin: A nanocarrier prepared by an adaptable microfluidic platform. **M. Alam**, J. Campagna, H. Rollins, P. Spilman, I. Nishimura, V. John

11:10 BIOT **690.** Encapsulation and release of dsDNA through dual-responsive, biodegradable hydrogel capsules. **B.A. Tucker**, J. Chen, V.A. Kozlovskaya, D.E. Graves, E.P. Kharlampieva

Section D

InterContinental San Francisco

Telegraph Hill

Quality by Design

Case Studies on Process Understanding & Design Space

J. Glassey, R. Godavarti, *Organizers*

P. Slade, A. Staby, *Presiding*

8:30 BIOT **691.** Successful mAb design space claim approach. **R. Hamilton**

8:50 BIOT **692.** Resin attribute and its interaction with process parameters to impact product quality and process performance for cation exchange chromatography. **A. Hagstrom**, S. Madaras, J. Prentice, S. Parra, O. Terova, G. Miro-Quesada, M. Stone, D. Robbins

9:10 BIOT **693.** Defining design space: Strategies to improve efficiency during process validation. **T. Peram**

9:30 BIOT **694.** Case study: Lifecycle management of a process wide design space. **A. Kleinjans**

9:50 Intermission.

10:10 BIOT **695.** Monte Carlo tool for prediction of variability in product quality attributes and definition of downstream process design space. **T.M. Wasylenko**, M. Coolbaugh, T. Dahal-Busfield, A. Kanodia, K. Kelly, N.M. Troccoli, Y. Waghmare, R. Patil, K.P. Brower, V. Warikoo

10:30 BIOT **696.** Mechanistic modeling of chromatography: An industry perspective and vision. **J. Griesbach**, F. Stueckler

10:50 BIOT **697.** Identification of key/non-key process and model parameters of autoinjector devices via global sensitivity analysis using mechanistic models. **P. Rolandi**, F. Schlegel

11:10 BIOT **698.** Design space characterization for filling process leveraging modeling and pilot scale capabilities. **M. Boggara**, V. Padmakumar, N. Rathore

Section E

InterContinental San Francisco

Sutter

Emerging Technologies

Cell & Gene Therapy

Y. Y. Chen, Y. Kim, J. P. Pieracci, *Organizers*

C. Beisel, E. Gschweng, *Presiding*

8:30 BIOT **699.** Immunotherapy using protein nanoparticles for improved response towards human cancer antigens. **M. Neek**, J. Tucker, N. Molino, E. Nelson, S. Wang

8:50 BIOT **700.** Engineering self-modulating T cells to prevent cytokine release syndrom in adoptive T-cell therapy. **M. Lin**, H. Kehoe, Y.Y. Chen

9:10 BIOT **701.** Drug responsive control systems for more potent and safer chimeric antigen receptor T cells. **B. Wang**

9:30 BIOT **702.** Evaluating cost-effectiveness of allogeneic T-cell immunotherapy based on a bioprocess economic model. **N. Razavilar**, K. Wallner, R. Pedroza, J. Delisle, C. McCabe

9:50 Intermission.

10:10 BIOT **703.** Data-fusion based process analytics for stem cell immunotherapy cell-culture on micro-carriers in bioreactor. S. Yoon, **B. Kuang**

10:30 BIOT **704.** Opportunities and challenges for vector manufacturing used for gene therapy. **S. Ozturk**

10:50 BIOT **705.** Efficient microRNA delivery system for treatment of disease by using cholesterol-conjugated microRNA and pegylated polycationic polymer. **B. Mun**, E. Jang, S. Han, J. Ki, H. Son, Y. Choi, Y. Huh, S. Haam

11:10 BIOT **706.** Histone-targeted gene transfer leads to enhanced MSC differentiation with 100-fold reduced BMP-2 dosing for bone regenerative applications. **E.V. Munsell**, M.O. Sullivan

Section F

InterContinental San Francisco

Grand Ballroom B/C

Biotechnology & Bioengineering Elmer Gaden Award Lecture

T. M. Przybycien, *Organizer, Presiding*

D. S. Clark, *Presiding*

11:30 BIOT **707.** Difficult-to-remove CHO host cell protein impurities. **K. Lee**

THURSDAY AFTERNOON

Section A

InterContinental San Francisco

InterContinental C

Downstream Processes

Advances in Non-Chromatographic Separations

A. Azevedo, R. Barros, V. Natarajan, N. Tugcu, *Organizers*

E. Benabaji, *Organizer, Presiding*

A. Azevedo, *Presiding*

2:00 BIOT **708.** Evolution of an improved high-throughput scale-down model for flocculation studies. **A. Radhamohan Keba**, J. Bill

2:20 BIOT **709.** Investigation of virus retention mechanisms by size exclusion membranes: The role of membrane properies and solution conditions in different flow regimes. **P. Kosiol**, C. Kahrs, B. Hansmann, M. Ulbricht, V. Thom

2:40 BIOT **710.** Evaluation of a new all-synthetic depth filter media demonstrates improved clarification and soluble impurity clearance post-protein A and low pH viral inactivation. **H.C. Nguyen**, A. Langland, B. Meyer, D.S. Kahn, J.A. Costanzo, J. Amara

3:00 BIOT **711.** Continuous precipitation of process related impurities from clarified cell culture supernatant using a novel Coiled Flow Inversion Reactor (CFIR). **N. Kateja**, H. Agarwal, A. Saraswat, M. Bhat, A.S. Rathore

3:20 Intermission.

3:40 BIOT **712.** Impact of novel continuous clarification techniques on sizing and optimization of depth filtration trains. **K. Galipeau**, M. Collins, E. Ayturk

4:00 BIOT **713.** Countercurrent staged diafiltration for monoclonal antibody formulation. **Y. Li**, A. Anirudh, A.L. Zydney

4:20 BIOT **714.** Adsorptive properties of filter aids. **O. Khanal**, N. Singh, S. Traylor, X. Xu, Z. Li, A.M. Lenhoff

4:40 BIOT **715.** Elucidate the effects of filtration conditions on virus removal. **X. Qian**, R. Fan, S. Wickramasinghe

Section B

InterContinental San Francisco

Grand Ballroom A

Drug Product & Delivery

Quality Assurance Challenges for Biopharmaceuticals: Single Use Processing Containers, Primary Packaging, Delivery Devices & Excipients

T. Randolph, E. Sahin, *Organizers*

C. Garvin, P. Paranjpe, C. Undey, *Presiding*

2:00 BIOT **716.** Activity of inactive ingredients: Foundations for innovations in drug excipients. **J. Pottel**, J. Irwin, B. Shoichet

2:20 BIOT **717.** Suitability and challenges of using Raman spectroscopy for polysrobate testing– use of Multivariate analysis to quantify variability. **E. Bolessa**, T. Wang, N. Deorkar, T. Wang

2:40 BIOT **718.** Nanobubble stability and protein aggregation in pharmaceutically-relevant formulations. **J. Snell**, T. Randolph

3:00 BIOT **719.** Excipient & pH targeting in bulk drug substance: A modified approach to buffer exchange during diafiltration. **R.W. Muthard**, G. Tran, A. Sophocleous, A.C. Dumetz, Y. Wu, K.E. Goklen

3:20 Intermission.

3:40 BIOT **720.** Performance of capping on residual seal force and container close integrity. **R. Ovadia**, P. Lam

4:00 BIOT **721.** Modeling plunger-stopper placement to optimize combination product process design. **J.P. Bernacki**, J. Jazayeri, D. Marsiglio, G. Gordon, N. Rathore

4:20 BIOT **722.** In-line Raman spectroscopy for bispecific assembly process monitoring. **A. Maier**

4:40 BIOT **723.** Development and implementation of an automated HIAC approach for high throughput subvisible particle analysis. **J. Purtell**, M. Berke, J. Yeary, E. Avanes, S. Cao, C. Ren, R. Kaushik

Section C

InterContinental San Francisco

InterContinental B

Quality by Design

Implementation & Description of Control Strategy

J. Glassey, R. Godavarti, *Organizers*

H. Shen, *Organizer, Presiding*

D. Robbins, *Presiding*

2:00 BIOT **724.** Continuous improvement of control strategy at Genentech and Roche. **A.S. Miller**

2:20 BIOT **725.** Practical considerations of knowledge management as an enabler of quality throughout the product lifecycle. **D. Paolella**, S. Weisser, P. Smith, A.R. Ubiera

2:40 BIOT **726.** Advanced process control strategy for consistent product quality and improved manufacturing efficiency. **C. Jiang**

3:00 BIOT **727.** Real-time monitoring of critical quality attributes and process parameters by spectroscopy during chromatographic capture and polishing steps. **M. Rudt**, N. Bestrich, D. Buchler, L. Rolinger, A. Sanden, J. Hubbuch

3:20 Intermission.

3:40 BIOT **728.** Exploring PAT approaches for ultrafiltration/diafiltration as the first step to continuous process design. **D. Arzensek**

4:00 BIOT **729.** Implementation of QbD for development of a downstream process for a therapeutic biosimilar. **A.S. Rathore**, R. Bhambure

4:20 BIOT **730.** Implementation of a QbD bioprocess into a traditional manufacturing site. **N.L. McKnight**, A. Kleeb, P. Walser

4:40 BIOT **731.** Automated methodology for post-approval management of a process control strategy. **P.R. Smith**, B.F. Marques, T. Wiley, K.E. Goklen

THURSDAY EVENING

Section F

InterContinental San Francisco

Telegraph Hill

Biotechnology & Bioengineering Daniel IC Wang Award

T. M. Przybycien, *Organizer, Presiding*

D. S. Clark, *Presiding*

5:00 BIOT **732.** Novel insights into understanding and designing regulatory RNAs. **L.M. Contreras**

BIOL

Division of Biological Chemistry

L. Hedstrom, *Program Chair*

SOCIAL EVENTS:
Social Hour, 7:00 PM: Sun, Tue

SUNDAY MORNING

Section A

Moscone Center

130

Graduate Student & Postdoctoral Fellow Symposium

L. Hedstrom, *Organizer*

M. E. Farkas, *Presiding*

8:30 Introductory Remarks.

8:35 BIOL **1.** RNA labeling induced by oxidation with high spacial resolution. **Y. Li**, R. Spitale

8:50 BIOL **2.** CRISPR-Cas9: Computational insights toward improved genome editing. **G. Palermo**, Y. Miao, R. Walker, M. Jinek, J. McCammon

9:05 BIOL **3.** Luminescence probes of deaminated nucleotide surveillance enzymes DUT and ITPA. **D. Ji**, Y. Pavlov, E.T. Kool

9:20 BIOL **4.** Monitoring the phenotypic response of FoxO1 at the single cell level in patient samples. **J. Simpson**

9:35 BIOL **5.** Identification of novel allosteric HSP72 inhibitors. **H. Traynor**, R. Burke, Y. Le Bihan, I. Collins, R.L. van Montfort

9:50 BIOL **6.** Polymerase-mediated synthesis of TNA polymers containing a fluorescent base that can read through G-repeats in a DNA template. **H. Mei**, C. Shi, J. Chaput

10:05 Intermission.

10:20 BIOL **7.** Antibiotic resistance evolved via inactivation of a ribosomal RNA methylating enzyme. **V. Stojkovic**, L. Noda-Garcia, D. Tawfik, D.G. Fujimori

10:35 BIOL **8.** Comparative analysis of translesion DNA synthesis by a high fidelity DNA polymerase. **A. Dasari**

10:50 BIOL **9.** Ultra-photostable, genetically directed fluoromodule enables STED nanoscopy and long time scale single protein tracks in live bacteria. **S. Saurabh**, A.M. Perez, C.J. Comerci, L. Shapiro, W.E. Moerner

11:05 BIOL **10.** Infrared spectroscopy reveals a base stacking limit in DNA G-quadruplexes. **D.A. Price**, Z.J. Kartje, T.D. Hill, G. Cairo-Baza, K.T. Gagnon, S.D. Moran

11:20 BIOL **11.** Synthesis, spectroscopic investigation, biological screening, interaction with SS-DNA and DFT study of aliphatic ferrocenyl ureas. **F. Asghar**, A. Badshah, I.S. Butler

‡ *Cooperative Cosponsorship*

Section B

Moscone Center
131

Ronald Breslow Award for Achievement in Biomimetic Chemistry: Symposium in honor of Benjamin G. Davis

B. G. Davis, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 BIOL **12.** Chemical Immunology - New approaches to study killer T-cell activation. **S. van Kasteren**

8:25 BIOL **13.** Immunomodulation by targeted delivery of carbon monoxide using artificial metalloproteins. **G. Bernardes**

8:45 BIOL **14.** Sulfur chemistry for biology and human health. **J.M. Chalker**

9:05 BIOL **15.** Chemical biology tools for studying the O-GlcNAc modification of proteins. **D.J. Vocadlo**

9:40 Intermission.

9:45 BIOL **16.** Controlling biological machines with synthetic photoswitches. **D. Trauner**

10:20 BIOL **17.** Mass spectrometry of membrane proteins - the lipid connection. **C. Robinson**

10:55 BIOL **18.** Homogeneous glycoproteins for structural and functional study. **C. Wong**

11:30 Introduction of Awardee.

11:40 BIOL **19. Award Address** (Ronald Breslow Award for Achievement in Biomimetic Chemistry

Sponsored by Ronald Breslow Award Endowment).

Sugars & proteins: Towards a synthetic biology. B.G. Davis

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

National Fresenius Award: Symposium in honor of Neal K. Devaraj

Sponsored by ORGN, Cosponsored by BIOL

Cellulose Structure & Biosynthesis

In the Plant Cell Wall

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

SUNDAY AFTERNOON

Section A

Moscone Center
131

Goodman Award: Symposium in honor of Jennifer Doudna

J. Doudna, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 BIOL **20.** CRISPR immune response to viruses that infect bacteria. **B. Wiedenheft**

2:50 BIOL **21.** Retooling CRISPR to turn genes on and off. **L. Gilbert**

3:35 BIOL **22.** CRISPRi/dCas9 for complex genome regulation and disease research. **L. Qi**

4:20 Introduction of Awardee.

4:25 BIOL **23.** CRISPR biology: Expanding nature's toolkit for genome engineering. **J. Doudna**

Section B

Moscone Center
3014/3016

ACS Award in Pure Chemistry: Symposium in honor of Neal K. Devaraj

N. K. Devaraj, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 BIOL **24.** Measuring and modulating the repair of DNA damage. **E.T. Kool**

2:35 BIOL **25.** Expanding the synthetic capabilities of yeast. **V.W. Cornish**

3:05 BIOL **26.** Transition metal signaling in the brain and beyond. **C.J. Chang**

3:35 Intermission.

3:55 BIOL **27.** Evolving click chemistry → SuFEx. **K.B. Sharpless**

4:25 Introduction of Awardee.

4:30 BIOL **28. Award Address** (ACS Award in Pure Chemistry sponsored by the Alpha Chi Sigma Fraternity & the Alpha Chi Sigma Educational Foundation). In situ synthesis and modification of lipid membranes. N.K. Devaraj

5:05 Concluding Remarks.

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Cellulose Structure & Biosynthesis

Evolution of Synthases & Fine Structure of Microfibrils

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Sponsored by INOR, Cosponsored by BIOL

SUNDAY EVENING

Section A

Moscone Center
West Hall

Current Topics in Biochemistry

L. Hedstrom, *Organizer*

7:00 - 9:00

BIOL **29.** Clarification by flocculation: A promissing solution for high cell density. **C. Decarnin**

BIOL **30.** Exploration of the N-terminal extension's role in human gamma-S crystallin function. **K. Roskamp**, A. Chenault, R. Martin

BIOL **31.** Chemical biology approach for dimethyllysine incorporation into proteins. **Z.A. Wang**, W. Liu

BIOL **32.** New tools for controlling the supramolecular assembly of proteins in living cells. **G.R. Casey**, X. Zhou, B. Xu, C.I. Stains

BIOL **33.** Structural analysis of heme c motifs for the template-based design of heme c proteins. **J. Kleingardner**

BIOL **34.** Unnatural lysine analogues to mimic the catalytic pocket of human DNA polymerase β. **C. Bhattacharya**, S.M. Daskalova, S. Hecht

BIOL **35.** Efficient method to study engineering temperature shift strategies for Chinese hamster ovary cell culture via mechanistic macroscopic kinetic modeling. **Y. Wang**, J. Xu, p. tang, s. liu, z. li

BIOL **36.** Investigating the specificity of methylated DNA binding by MBD1 and mutant peptides for transcriptional regulation. **S. Scherer**, A. Stewart

BIOL **37.** Synthesis and evaluation of a norbornene containing substrate for protein farnesyltransferase. **J. Wollack**, J. Rowe, C. Sutton, L. Crepeau, K. Caron, M.D. Distefano

BIOL **38.** Developing a pipeline for generating TNA-phosphoramidite and TNA-triphosphate monomers for the *in vitro* evaluation of the properties of the polymers. **S. Bala**, J. Liao, J. Chaput

BIOL **39.** Exploring the role of Tat-SF1 as an HIV-1 host factor. **M. Warrick**, H.B. Miller

BIOL **40.** Mutational studies of a deoxyribozyme by high-throughput sequencing. **D. Venugopal**, S. Kobori, Y. Yokobayashi

BIOL **41.** Transcriptiome-wide mapping of RNA-RNA interactions. **M. Oumais**, A. Luptak

BIOL **42.** Possible prebiotic fabrication of ribonucleotides using microdroplets. **I. Nam**, J. Lee, H. Nam, R.N. Zare

BIOL **43.** Tat-specific factor 1's role in HIV RNA stability. **A.P. Goodwin**, H.B. Miller

BIOL **44.** Theoretical characterization of the H-bonding and stacking potential of two nonstandard nucleobases expalnding the genetic alphabet. **M. Chawla**, **R. Oliva**, **L. Cavallo**

BIOL **45.** Live cell imaging of RNA using endogenous fluorophore protoporphyrin IX. **D. Zhang**

BIOL **46.** ADARs and RNA; Structual basis for site selectivity of ADAR2. **J. Thomas**, M. Matthews, Y. Zheng, P.A. Beal, A.J. Fisher

BIOL **47.** Nucleobase analogs as probes for substrate recognition and repair by DNA glycosylase MutY. **C. Majumdar**, S.S. David, A. Manlove

BIOL **48.** Bioorthogonal near-infrared fluorogenic probe for mRNA detection. H. Wu, S.C. Alexander, **S. Jin**, N.K. Devaraj

BIOL **49.** Bioluminescent detection of HIV persistency via a stem-loop probe. **B. Cherif**, A. Moutsiopoulou

BIOL **50.** Optimizing the production of FOXA2 to unravel the interaction between homeodomain and Forkhead transcription factors. **S. Ramirez**

BIOL **51.** Investigation into the broad substrate specificity of the DNA glycosylase hNEIL1. **B. Anderson**, J. Ashby, A.M. Fleming, C.J. Burrows, S.S. David

BIOL **52.** Influence of loop mutations on G-quadruplex unfolding. **B.A. Tucker**, J.S. Hudson, D.E. Graves

BIOL **53.** Oncostatin M mediated regulation of microRNA-21 function in HeLa cells. **N. Jain**, S. Ahmed, **M.J. Sever**

BIOL **54.** 5′ Start site heterogeneity of the HIV-1 RNA and its effect on structure and function. **D. Francis**, M. Orellana, J. Brown, M. Summers

BIOL **55.** Parallel stranded G-quadruplex composed of Threose Nucleic Acid (TNA). **J. Liao**, I. Anosova, S. Bala, W.D. Van Horn, J. Chaput

BIOL **56.** Structural stability analysis of a S. cerevisiae DEAD-box protein. **Z. Iezzi**, C. Bardine, H. Englert, I. Garcia

BIOL **57.** High-throughput mutational analysis and engineering of self-cleaving ribozymes by sequencing. **S. Kobori**, Y. Yokobayashi

BIOL **58.** Elucidation of the role of adenine DNA glycosylase mutyh in MNNG-mediated cell cytotoxicity. **D.M. Banda**, A.G. Raetz, G. Xu, X. Ma, P.L. McKibbin, A. Rajavel, C.B. Lebrilla, S.S. David

BIOL **59.** Synthesis and screening of a naphthalene diimide bisintercalator library. **E. Gratton**, B.L. Iverson

BIOL **60.** High-yield syntheses of DNA duplexes containing interstrand cross-links at a single well-defined location via a reductive amination reaction between 2-aminopurine and an abasic site. **M. Imani Nejad**, N.E. Price, Y. Wang, K.S. Gates

BIOL **61.** Engineering the N-terminal domain of pyrrolysyl-tRNA synthetase: Optimizing genetic incorporation of non-canonical amino acids. **V. Sharma**, W. Liu

BIOL **62.** Complete Zn2+ linchpin coordination sphere of the DNA repair glycosylase MUTYH. **N. Nunez**, S.S. David, J.B. Siegel, C. Lim

BIOL **63.** Enzymatic site-specific labeling with RNA-TAG for affinity purification of RNA-protein complexes. **K.N. Busby**, N.K. Devaraj

BIOL **64.** 5-Hydroxymethylcytosine impacts Holliday junction structure to promote recombination via endonuclease G. **C. Vander Zanden**, R.K. Rowe, A.J. Broad, A.B. Robertson, P.S. Ho

BIOL **65.** Ligand selectivity in a pathogenic preQ1 riboswitch aptamer domain. **K.M. Yamakawa**, M. Doan, J.M. Davison, M.N. Pahl, I.T. Suydam

BIOL **66.** E2F1 and p27 regulation in non-neuronal cells by isoxazole 9. **M. McCabe**, **M.J. Sever**

BIOL **67.** Structural and energetic characterization of the emissive RNA alphabet based on the isothiazolo[4,3-d]pyrimidine heterocycle core. M. Chawla, R. Oliva, **L. Cavallo**

BIOL **68.** Interaction of Menaquinone (MK) analogs (MK-1 and MK-2) with phospholipids. **G. Cardiff**, B.J. Peters, J.T. Koehn, J.B. Hough, A. Groninger, D.C. Crick, D.C. Crans, F. Fontes

BIOL **69.** Ca2+ induced conformational changes of calmodulin and troponin C chimera. **C. Wei**, D. Jensen, K. Schafer, E.A. Fabry

BIOL **70.** Selective detection of protein homologues by outer membrane protein G nanopore. **B. Yang**, M.A. Fahie, H. Wang, P. Limpikirati, R.W. Vachet, S. Thayumanavan, M. Chen

BIOL **71.** How host gender affects the polysaccharide capsule of *Cryptococcus neoformans*. **P. Doski**, E. McClelland

BIOL **72.** Structure of the pro-apoptotic BCL-2 family protein BAD and insight into BAD-calcineurin interactions. **S.N. Blakeney**, E.C. Cook, T.P. Creamer

BIOL **73.** Aquaporin inspired water purification membrane based on graphene oxide membrane. **C. Lee**, D. Kim, G. Lee, Y. Lee, Y. Lee

BIOL **74.** Amyloid Forming Sequences in *Trichomonas vaginalis*. **A. Asakawa**, C. Chan

BIOL **75.** Exploration of the interactions of hen egg white lysozyme with deoxyribonucleic acids. **E.A. Fabry**, C. Wei, T. Shields

BIOL **76.** Proteomics-based screening and identification method for redox sensitivities of global cellular cysteine residues. **K. Araki**, K. Fukui, T. Natsume

BIOL **77.** Functionalization of polydopamine via the Aza-Michael reaction for antimicrobial interfaces. **P.T. Ha**, C. Huang, C. Liu, Y. Huang

BIOL **78.** Utilization of extracts of garlic, oregano, neem and a commercial insecticide on endophyte bacteria on orange leaves infected by *citrus greening*. **J. Becerra Lopez**, **A. Perez Matos**

BIOL **79.** Characterization of the huntingtin aggregation pathway via single-molecule and super-resolution fluorescence microscopy. **C. Becker**, **R. Harman**, **A. Khan**, R. Levy, W.C. Duim

BIOL **80.** Is it a biological response or chemical process? Chemical and transcriptional regulation experiments probe the cause for the increased accumulation of Chlorogenic Acid (CGA) in carrot root slices exposed to UV-B light. G.E. Bartley, R.J. Avena-Bustillos, W. Du, M. Hidalgo, B. Cain, **A.P. Breksa**

BIOL **81.** N acetyl cysteine as an inducer of retina regeneration. **J. Landers**, K. Del Rio-Tsonis, N. Echeverri

BIOL **82.** 5-azidomethyl-2'-deoxyuridine triphosphate can be efficiently incorporated by a repair DNA polymerase. **C. Garcia**, Y. Ren, Z. Wen, S.F. Wnuk, Y. Liu

BIOL **83.** Comparison of synthetases in the incorporation of the non-natural amino acid p-azidophenylalanine in the oncogenic protein kRas. **M. Wheeler**, T. Andresson, R.E. Connor

BIOL **84.** Precise delivery of a chemotherapeutic Prodrug to mitochondria of prostate cancer cells to bypass repair induced resistance. **U. Basu**

BIOL **85.** Visualizing the chain-flipping mechanism to study inhibition and protein-protein interaction in fatty acid biosynthesis. **K. Charov**, J. Beld, M.D. Burkart

BIOL **86.** Assessing cysteine residue thiol status in T-Darpp, a protein involved in chemoresistance. **J.A. Aldana-Mendoza**, **P. Farias**, J. Momand

BIOL **87.** Nanomaterials toxicological evaluation: Natural product shielded magnetite nanoparticles. **H. Huang**, J.L. Liu, S. Bashir

BIOL **88.** Analogs of methyl 4-(4-chlorophenyl)-4-oxobut-2-enoate that inhibit MenB in the bacterial menaquinone biosynthesis pathway. **Y. Si**, J. Matarlo, F. Daryaee, P.J. Tonge

BIOL **89.** Characterization of a robust serine protease from *P. intermedia*. **S. Spradlin**, C.M. Evilia

BIOL **90.** Reverse transcription past major guanine oxidation products in RNA. **A. Alenko**, A.M. Fleming, C.J. Burrows

BIOL **91.** Importance of F365 in the binding of inhibitors in *Escherichia coli beta-glucuronidase*. **S. Van Shufflin**

BIOL **92.** Ratiometric fluorescent chloride sensor. **K. VanDenburgh**, Y. Liu, B. Qiao, A.H. Flood

BIOL **93.** Highly selective small potassium transporter induces cancer cell death. **F. Shen**, D. Yang

BIOL **94.** Evaluating the effect of lipophilicity on antimicrobial potency, cytotoxicity, and combinatorial library design. **J.A. Turkett**, K. Bicker

BIOL **95.** Determinants of the pKa value of catalytic residue in de novo designed enzymes. K. Hiebler, C. Castaneda, **O. Makhlynets**

BIOL **96.** Allosteric control of histone demethylase KDM5A. **J.E. Longbotham**, C. Chio, M. Kelly, D.G. Fujimori

BIOL **97.** Pathological mutations in the prion protein modulate the metal driven cis interaction. **G.P. Roseman**

BIOL **98.** Electrophilic reactive carbonyl species: Participation in the nonenzymatic covalent protein modification of human hemoglobin. **P. Ropski**, J. Pattan, B. Park, R.W. Holman, K. Rodnick

BIOL **99.** Towards a mechanistic understanding of nonenzymatic glycation of human hemoglobin: Diverse effects of inorganic phosphate on the initial noncovalent binding of glucose. **A. Hendricks**, **C. Mottishaw**, J. Mitchell, P. Ropski, B. Smith, G. Titus, B. Park, M. Finkbeiner, R.W. Holman, K. Rodnick

BIOL **100.** Fine-tuning triazabutadiene stability for controlled aryl diazonium release. **L. Guzman**, J.C. Jewett

BIOL **101.** Self-Assembling nanoluciferase fragments as probes for alpha-synuclein solubility. **T. Truong**, C. Bilyeu, J. Zhao, T. Nelson, C.I. Stains

BIOL **102.** Effects of DNA bending on T=C CPD deamination. **K. Wang**, J.S. Taylor

BIOL **103.** Development of targeted stigmasterol-solid lipid nanoparticles by hyaluronic acid and transferrin for lung cancer therapy. **Z. Torres**, Y. Delgado, K. Griebenow

BIOL **104.** Use of infrared spectroscopy to study the structural changes of calreticulin upon the addition of ligand. **A. Farquharson**, C. Thomas, L. Maynard

BIOL **105.** Withdrawn.

BIOL **106.** Cyclopropene neurotransmitters for biorthogonal imaging of neural circuits. **P. kumar**, S. Li, D. Shukhman, S.T. Laughlin

BIOL **107.** Effect of caffeine on lipophagy in mammalian skeletal muscle cells. **D.S. Enyart**, J. Stansell, J.V. Ruppel, S. Kinsey, B. Baumgarner

BIOL **108.** Use of CDNB assay to determine calreticulin domain responsible for autoacetylation. **C. Nnebe**, C. Thomas, L. Maynard

BIOL **109.** Design of biomimetic antimicrobial peptide-polymer conjugates as building blocks for reactive/responsive membranes: A water purification approach. **V. Ortiz Gomez**, V. Rodriguez, E. Nicolau

BIOL **110.** Effect of 4,4' DDT, 4,4' DDE, 4,4' DDD, and 2,4' DDD on dihydrotestosterone binding to and releasing from the androgen receptor. **T. Resto**, F. Dean, A. Chavez, V. Flores

BIOL **111.** Synthesis and evaluation of Nebraska red derivatives for protein labeling studies. **L. Lesiak**, X. Zhou, C.I. Stains

BIOL **112.** Tryptophan derivatives as novel fluorescent probes for studying protein conformational changes and DNA–protein interaction. **P. Talukder**, S. Chen, B. Roy, P. Yakovchuk, S. Hecht

BIOL **113.** Photo-uncaging of reactive species and fluorescence with visible light and NIR. **S. Dai**, D. Yang

BIOL **114.** Withdrawn.

BIOL **115.** Molecular dynamics simulations of metabolite fibrils. **P. Rehak**, L. Vukovic, P. Kral

BIOL **116.** Physiological and behavioral adaptations of *Vibrio cholerae* to fatty acids in a continuous culture (bioreactor) model. **R.A. Boeger**, A. Turgeson, D. Giles, B. Harris

BIOL **117.** Binding mechanism study of coomassie brilliant blue species and bovine serum albumin. **R.N. Ngo**, C. Wei, E.A. Fabry

BIOL **118.** Using comb-branched DNA to construct deoxyribozyme-based biosensors. **M.R. Polaske**, E. Teselle, D.A. Baum

BIOL **119.** Effects of heterocyclic diamidine antiparastitic agent binding to DNA on restriction enzyme kinetics. **T.M. Rodriguez**, S.A. Winkle

BIOL **120.** Developing FRET assays to study the binding and regulation of fibroblast growth factor to its receptor. **M. Mohale**

BIOL **121.** Mechanistic studies of StyA1 styrene monooxygenase from *Rhodococcus Opacus*. **J.L. Diaz**, G.T. Gassner, d. Tischler

BIOL **122.** Development of a fluorescence polarization assay for RhlI. **N.R. Rexrode**, J. Taffin, N. Lam, R. Nagarajan

BIOL **123.** Bioluminescence and photoluminescence properties of the earthworm *Eisenia lucens*. **P. Taborsky**, O. Pes

BIOL **124.** Toward Raman-based diagnostics for amatoxins: Synthetic, computational, and spectroscopic studies on analogs for the substituted tryptathionine sulfoxide core of amanitins, the peptide toxins of *Amanita phalloides*. **K. Yniguez**, T.G. Moreno, A. Ringer McDonald, S.C. Eagon, E. Jones

BIOL **125.** Hyper obesity suppression by the products of *Rhinacanthus nasutus*: A study in rats. **T. Kedam**

BIOL **126.** Energy depletion in vitro potentially caused immunosuppression: A multi-omics characterization of pathogenic threat in spaceflight. **N. Chakraborty**, A. Cheema, A. Gautam, S. Miller, A. Hoke, M. Jett, R. Hammamieh

BIOL **127.** Structural analysis of tau peptide interactions with lipid membranes using Fourier transform infrared spectroscopy. **P. Engen**, L. Masterson

BIOL **128.** Growth based complementation assay in *E. coli* for inhibitor screening of *S-adenosylmethionine synthetase*. **G.G. Parungao**, R.M. Blumenthal, R.E. Viola

BIOL **129.** Effect of the antimicrobial peptide combi-2 on vesicles of membrane mimicking systems of normal and cancer cells. **B.M. Almarwani**, A. Sunda-Meya, N. Phambu

BIOL **130.** Quantification of the minimum numbers of TLR2 agonists necessary to elicit a detectable immune response. **W.J. Howitz**, B. Moser, A. Esser-Kahn

BIOL **131.** Development of a novel, neural-activity triggered split enzyme. **B. O'Neill**, S. Laughlin

BIOL **132.** Enzyme-enzyme proximity stimulates iNOS activity. **K.M. Fomchenko**, D.J. Hirsh

BIOL **133.** Investigating the conformational landscape in a signaling protein complex with optical tweezers. **J.P. England**

BIOL **134.** Reactivity of bovin serum albumin with ligands of cisplatin analogs. **N.C. Puckett**, K. Williams

BIOL **135.** Selective in vivo cell labeling mediated cancer targeting. H. Wang, **K. Cai**, R. Wang, J. Cheng

BIOL **136.** Withdrawn.

BIOL **137.** *In vitro* biochemical studies of the midgut serine protease AaSPVII of the Zika vector *Aedes aegypti*. **J.T. Nguyen**, A. Rascon

BIOL **138.** Withdrawn.

BIOL **139.** Elucidating the temporal dynamics of caspase activity within the mitochondrial pathway of apoptosis. **R.D. Reif**, S. Morris

BIOL **140.** Charaterization of menaqinone-2. **E. Magallanes**, J.T. Koehn, B.J. Peters, C.N. Beuning, M. Zhu, D.C. Crick, D.C. Crans

BIOL **141.** Allosteric inhibition via two-step enzyme isomerization of human herpesvirus protease protein-protein interaction decreases viral infectivity of Kaposi's sarcoma-associated herpesvirus in mammalian cells. **T. Acker**, J. Gable, M. Bohn, P. Jaishankar, A.R. Renslo, C. Craik

BIOL **142.** Chemical imaging of neuron-astroglia interactions. **A. Preston**, J. Farr, S. Laughlin

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

BIOL **143.** Computational study of relative thermodynamic stability of mutant base pairs between keto, enol and deprotonated forms of guanine and thymine at DNA polymerase active site. **S.N. Maximoff**, J. Eloge, S. Kamerlin, J. Florian

BIOL **144.** Dipyrimidine sequence library for determining the sequence dependence of UV-induced *cyclobutane pyrimidine dimer* formation. **C. Lu**, J.S. Taylor

BIOL **145.** Direct observation of breathing dynamics at the mismatch induced DNA bubble by smFRET measurement. **T. Paul**, P. MIshra

BIOL **146.** DNA Editing in DNA/RNA hybrids by adenosine deaminases that act on RNA. **Y. Zheng**, C. Lorenzo, P.A. Beal

BIOL **147.** Probing RNA recognition by human ADAR2 using a high-throughput mutagenesis method. **Y. Wang**, P.A. Beal

BIOL **148.** Successful screening of aptamers for an early diagnosis of a periodontitis. **B. Lee**, J. Park, Y. Ko, M. Gu

BIOL **149.** Single-molecule FISH of specific mRNAs using click chemistry. **S.H. Rouhanifard**, A. Raj

BIOL **150.** Dynamics of the *E. coli* beta clamp and its influence on DNA loading. **B. Koleva**, J. Baez, J. Conway, A. Wu, P.J. Beuning

BIOL **151.** T4 DNA ligase-catalyzed polymerization of modified oligonucleotides: Discovery and application of a high-fidelity codon set to the evolution of modified aptamers. **Y. Lei**, D. Kong

BIOL **152.** Design and synthesis of thiol cleavable self-immolative linkers and their conjugation to proteins. **C.M. Sadlowski**, N. Murthy

BIOL **153.** Tools for controlled microdomain formation and protein localization in artificial phospholipid membranes. **A.K. Rudd**, N.K. Devaraj

BIOL **154.** Site-Specific nanocluster synthesis in biomolecular hosts. **S. Teymorian**, A. West, M. Griep

BIOL **155.** Fourier transform infra red spectroscopy based spectral biomarker identification: Applications in classifying lung cancer subtypes. **A. Sarkar**, A. Sadhu, S.B. Thakur

BIOL **156.** Withdrawn.

BIOL **157.** ROS responsive self-cyclization for hydroxyl radical detoxification. **J. Liu**, S. Abdul Salam, H. Zhu, E.J. Merino

BIOL **158.** New design for twin reactive oxygen species activated anti-tumor agents. **H. Zhu**, S. Abdul Salam, J. Liu, E.J. Merino

BIOL **159.** Investigation of catalytic activity of stable β-keto-acyl-ACP substrate analogs in quorum sensing signal synthesis. **N. Lam**, D. Dudekula, I. Csik, N. Collingwood, E.C. Brown, R. Nagarajan

BIOL **160.** Examination of essential genes involved in the biosynthesis of key metabolite by *Chlamydia trachomatis*. **T. Nguyen**, D.G. McCafferty

BIOL **161.** Versatile site-specific modification of native protein N termini using a panel of engineered peptide ligases. **A. Weeks**, J.A. Wells

BIOL **162.** Role of miRNAs in chick retina regeneration. **N.G. Burns**, A. Luz-Madrigal, J. Shi, S. Sreeskandarajan, L. Liu, P. Tsonis, C. Liang, K. Del Rio-Tsonis

BIOL **163.** Novel porphyrin derivatives for photodynamic therapy. **T.E. Hayes**, T. White, M.E. Scarbrough, J.E. Bradshaw

MONDAY MORNING

Section A

Moscone Center

131

Nucleic Acid Therapeutics: Mechanisms & Applications

M. Manoharan, *Organizer*

M. J. Damha, *Presiding*

8:00 Introductory Remarks.

8:10 BIOL **164.** Design and assembly of artificial proteins using nucleic acid hybridization. **J. Wengel**

8:45 BIOL **165.** This is your brain on antisense oligonucleotides: Distribution, activity and application to the treatment of severe neurodegenerative disease. **E.E. Swayze**

9:20 BIOL **166.** Applying the chemist's toolbox for studying nucleic acid structure and function. **M.J. Damha**, H. Abou Assi, D. O'Reilly, E. Malek-Adamian, M. Habibian, D. Vlaho, J. Bogojeski, S. Jana, S. Martinez-Montero, C. Gonzalez

9:55 Intermission.

10:10 BIOL **167.** Advances in RNAi therapeutics: Chemistry, mechanism and applications. **M. Manoharan**

10:45 BIOL **168.** Structure-based insights into stability, activity and protein interactions of chemically modified oligonucleotides. **M. Egli**

Section B

Moscone Center

132

Early Career Investigators in Biological Chemistry

L. Hedstrom, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 BIOL **169.** Withdrawn.

8:55 BIOL **170.** Introduction of D-glutamate at a key site of Aβ42 stabilizes a soluble aggregation intermediate and enhances toxicity. **J.A. Raskatov**, C.J. Warner, S. Dutta, A. Foley

9:15 BIOL **171.** Human monomeric insulin derived from cone snail venoms. **D. Chou**

9:35 BIOL **172.** Chemically modified macrophages for cancer imaging and drug delivery. M. Mingroni, J.J. Elliott, J. Hardie, **M.E. Farkas**

9:55 Intermission.

10:05 BIOL **173.** Development of peptide-based tools to study quorum sensing in streptococci. Y. Yang, B. Koirala, C.R. Bikash, N.R. Phillips, L.A. Sanchez, S.R. Hamry, **Y. Tal-Gan**

10:25 BIOL **174.** Chemical biology strategies illuminating how the proteostasis network modulates evolutionary excursions in sequence space by RNA viruses. **M. Shoulders**

10:45 BIOL **175.** Profiling endogenous protein phosphatase activity using direct activity probes. **C.I. Stains**

11:05 BIOL **176.** Pushing click chemistry to its limits: An in-vitro sample generation pipeline for high-throughput single-molecule FRET-based screening of proteins and ribosome-bound nascent chain libraries. **K.M. Hamadani**, P. Wu, J. Cate, S. Marqusee

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Cellulose Structure & Biosynthesis

Mechanism of Synthesis

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

MONDAY AFTERNOON

Section A

Moscone Center

131

Nucleic Acid Therapeutics: Mechanisms & Applications

M. Manoharan, *Organizer*

M. Egli, *Presiding*

1:00 Introductory Remarks.

1:05 BIOL **177.** New roles for G-quadruplexes in gene expression and infectious disease. **C.J. Burrows**, A. Fleming, Y. Ding

1:40 BIOL **178.** Advances in the chemistry of microRNA-based therapeutics. **C. Allerson**

2:15 Intermission.

2:30 BIOL **179.** Potent delivery of LUNAR™ nanoparticles containing synthetic mRNA for therapeutic protein expression. **P. Chivukula**

3:05 BIOL **180.** Homologous DNA recombination in vivo with the delivery of Cas9 ribonucleoprotein and donor DNA complexed to gold nanoparticles. **K. Lee**, M. Conboy, F. Jiang, H. Kim, M. Dewitt, H. Park, J. Corn, J. Doudna, I. Conboy, N. Murthy

Rising Star Award Symposium

Sponsored by WCC, Cosponsored by BIOL and PRES

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

Cellulose Structure & Biosynthesis

Synthase Trafficking & Synthesis of plant (1->3),(1->4)-D-glucans

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

L. Hedstrom, *Organizer*

8:00 - 10:00

32, 34, 48, 92, 106, 133, 135, 141, 161. See previous listings.

203, 206, 228, 256, 279, 292, 318, 321, 324. See subsequent listings.

TUESDAY MORNING

Section A

Moscone Center

131

Metalloprotein-Initiated Signaling Transduction Response to Redox Stress

Cosponsored by INOR

A. Liu, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 BIOL **181.** Screening of small molecule inhibitors of human pirin. **H. Osada**

8:40 BIOL **182.** Enzymology of hydrogen sulfide signaling. **R. Banerjee**

9:15 BIOL **183.** Probing heme trafficking, signaling, and dynamics in health and disease. **A.R. Reddi**

9:50 Intermission.

10:00 BIOL **184.** Enzyme mechanism-driven DNA-protein crosslinks during attempted DNA repair. **B. Demple**

10:35 BIOL **185.** Signal transduction mechanisms in heme-dependent gas-sensing transcription factors. **J.N. Burstyn**, J.P. Hines, H. Bowman, M.R. Dent, D.J. Stevens

11:10 BIOL **186.** How metal-dependent oxidation can redirect AAA+ proteases to new protein substrates. B. Ah, B. Brown, S. Calmant, J. Kardon, **T. Baker**

Section B

Moscone Center
132

Chemical Epigenetics

D. G. Fujimori, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 BIOL **187.** Advanced chemical genetics for epigenetics: Bump-and-hole and PROTACs. **A. Ciulli**

9:05 BIOL **188.** Regulation of catalysis and novel inhibitor chemotypes for histone demethylases. **D.G. Fujimori**

9:35 BIOL **189.** Discovery of A-395: A novel protein-protein interaction inhibitor of EED. **B. Pappano**

10:05 Intermission.

10:20 BIOL **190.** Development of irreversible small molecule epigenetic modulators to block menin-MLL in cancer. **J.E. Grembecka**, D. Borkin, S. Klossowski, H. Miao, K. Kempinska, J. Pollock, T. Purohit, B. Wen, D. Sun, T. Cierpicki

10:50 BIOL **191.** On the mechanisms of generation, recognition, and erasure of DNA and histone modifications. **X. Cheng**

Cellulose Structure & Biosynthesis

Biochemistry & Cellular Biology

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Sponsored by INOR, Cosponsored by BIOL

TUESDAY AFTERNOON

Section A

Moscone Center
131

ACS Chemical Biology Award Symposium

Cosponsored by WCC

A. Weidmann, *Organizer*

L. L. Kiessling, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 BIOL **192.** Profiling acetyltransferases to understand cancer's metabolic cues. **J.L. Meier**

2:35 BIOL **193.** Privileged First-Responding redox sensors in isozyme-specific apoptosis regulation. **Y. Aye**

3:05 BIOL **194.** Chemical tools for probing bacterial peptidoglycan activation of the innate immune system. **C.L. Grimes**

3:35 BIOL **195.** Cross-reactive cysteine modifications. **B.R. Martin**

4:05 Introduction of Awardee.

4:10 BIOL **196.** Activity-based proteomics – protein and ligand discovery on a global scale. **B.F. Cravatt**

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Sponsored by INOR, Cosponsored by BIOL

TUESDAY EVENING

Section A

Moscone Center
West Hall

Current Topics in Biochemistry

L. Hedstrom, *Organizer*

7:00 - 9:00

BIOL **197.** Label free proteomics profiling unveils downregulation of thrombin mediated signaling and aggregation of human platelets upon treatment with thrombin inhibitors. **C.C. Clement,** A. Babinska, J. Gonzalez

BIOL **198.** Allostery and catalysis of UDP-sugar pyrophosphorylases suggest a new approach to anti-parasitic treatments. J.T. Cramer, J.I. Führing, F.H. Routier, A. Lamerz, J. Schneider, P. Baruch, R. Gerardy-Schahn, **R. Fedorov**

BIOL **199.** Development of novel substrate inhibitors of bacterial phospholipid biosynthesis as new antibacterial agents. **P. Saklani**, **J. Luo**, D.P. Brown

BIOL **200.** Analysis of chemotypes in retail *Cannabis strains*. R.M. Hyslop, **C.E. Brown**, A. Schwabe, S. Desa, M. McGlaughlin

BIOL **201.** Novel application of TEC-disulfide replacement showcased in the synthesis of SFTI-1. **J. Barbaretta**, A.J. Wommack

BIOL **202.** Self-assembled synthetic ion channels. **D. Yang**

BIOL **203.** Discovering and manipulating miRNA biology utilizing click-chemistry. **D. Lorenz**, A. Garner

BIOL **204.** Synthesis & spectroscopic characterization of xenometabolite, biomarkers for the diagnosis of fatty acid β-oxidation disorder. **H.F. Sobhi**, S. Adams, M. Ekwuru, P. Teasley

BIOL **205.** Study of aminoglycosides binding to mitochondrial rRNA. **L. Garmo**, P. Madubashitha, E. Jones, C.S. Chow

BIOL **206.** Bioorthogonal metal catalysed transformation of dehydroalanine in peptides and proteins. **A. de Bruijn**, G. Roelfes

BIOL **207.** *In vitro* anti-neoplastic activity of specific phytocannabinoids of *Cannabis sativa*. **R.M. Hyslop**, A. Saviola, S. Bydalek, C.E. Brown, S. Desa, M. Thomas, A. Magiotta, S. Mackessy, C. Hansen, M. Brown

BIOL **208.** Quantifying the relative amounts of PrP polymorphisms present in prions isolated from heterozygous prion-infected animals. **C.J. Silva**, M.L. Erickson-Beltran, C. Hui, J.J. Badiola, J.R. Requena, R. Bolea

BIOL **209.** Novel application of scaffold treatment procedure with minimum side effects by using an engineered biodegradable scaffold. Y. Lo, G. Ren, E.J. Parish, **H. Honda**

BIOL **210.** Novel approaches to the developmental relationship of retinol binding protein and clinical phenotype of coronary heart disease. L. Lv, E.J. Parish, **D. Ren**, **G. Ren**, **H. Honda**

BIOL **211.** Novel application of new methodology in the treatment of enzyme as a preparation method for biocompatible material. G. Ren, E.J. Parish, Y. Lo, **H. Honda**

BIOL **212.** *In vitro* activation of purified *Aedes aegypti* mosquito wild-type Early Trypsin (AaET) versus the inactive AaET mutant. **R.M. Lucero**, A. Rascon

BIOL **213.** Importance of Ser26 in the folate half-reaction of *E. coli* MTHFR. **R. Li**

BIOL **214.** Interfacial interactions of glycine and short glycine peptides in confined spaces. **K. Doucette**, P. Chaiyasit, D.L. Calkins, K. Martinez, M.J. Fisher, D.C. Crans, A. Tongraar

BIOL **215.** Developing small molecule adjuvants from contact allergens. **S. Kim**, A. Esser-Kahn

BIOL **216.** Synthesis of 2-Arachidonoylglycerol: An endocannabinoid with potential as an anti-cancer drug. **S. Bydalek**, R.M. Hyslop

BIOL **217.** Purification and characterization of adenosine aminohydrolases from *Pisum Sativum*. **L. Thicklin**, P.C. Kline

BIOL **218.** Photoactivatable innate immune receptor for optogenetic inflammation. **B. Moser**, A. Esser-Kahn

BIOL **219.** Investigation of Cu(II) complexation with fourth microtubule-binding repeat of tau protein by ESI-MS, IMS-MS and NMR. **S. Ahmadi**, S. Zhu, R. Dutta Majumdar, R. Soong, D. Wilson, A. Simpson, H. Kraatz

BIOL **220.** Conformational sampling and non-dimer aggregates of HIV-1 protease containing darunavir promoted mutations. **L. Pham**, Z. Liu, L. Hu, X. Huang, A. Bhatt, K. Bentz, T. Tran, D. Savin, R. McKenna, G. Fanucci

BIOL **221.** Synthesis of fluorogenic phosphatidylcholine derivatives for kinetic studies of phospholipase A2 enzymes. **L. Zelaya**, J. Hajdu, T.G. Minehan

BIOL **222.** Enhancing efficacy of protease drugs through site-directed mutagenesis. **A. Amorello**, A. Batt, T. Baird

BIOL **223.** Investigating a new paradigm in melanocortin signaling and energy balance. **V. Chen**

BIOL **224.** Affinity ligand purification for pyridine dinucleotide binding proteins. **D. Andy**, J. Slama, T. Walseth

BIOL **225.** Elucidating Met18 functionality in iron-sulfur cluster biogenesis pathway. **C. Lee**, A. Vo, J. Cosman, D. Perlstein

BIOL **226.** Engineering a polymerase for accurate bypass of damaged DNA samples. **T. Coulther**, P.J. Beuning, M.J. Ondrechen

BIOL **227.** Topology study of one CpTat component, Hcf106, in resting and precursor binding state. **A.G. Habtemichael**, G. Thomas, C. Dabney-Smith

BIOL **228.** Single molecule imaging of protein activity in living cells. **N. Pinkin**, J. Smith, B. Liu, C.J. MacNevin, K.M. Hahn

BIOL **229.** Assessing the functionality of active site threonine substituted trypsin with disulfide residue serine variants. **J. Schuder**, B. Caswell, T. Baird

BIOL **230.** HPLC analysis of sulfation of dopamine derivatives by SULT1A3. **K. Reed**, J. Rogowiec, M.L. Cafiero, L.W. Peterson

BIOL **231.** Cloning of IME4 to establish a new model system to probe N6-methyladenosine modification of mRNA. **A. Barnaby**, C. Schoose, J. Dunkle

BIOL **232.** Gene expression in a synthetic tissue of artificial cells. **H. Niederholtmeyer**, N.K. Devaraj

BIOL **233.** Cobalticinium derivatives as mediators for bioelectrochemical catalysis with P450. **W. Bae**

BIOL **234.** Characterization of Sup35, Rnq1, and Ure2 cotranslational prion aggregation in *Saccharomyces cerevisiae*. **B.T. Allwein**, D. Cameron

BIOL **235.** Construction of hydrophobic nanoparticles based surface plasmon resonance biosensor for lysozyme detection. **Y. Saylan**, F. Yilmaz, A. Derazshamshir, A. Denizli

BIOL **236.** Photoswitchable immunostimulants for optical control of TLR activity. **A. Love**, T.J. Albin, A.P. Esser-Kahn

BIOL **237.** Solid phase peptide cyclization and development of PRC2 Inhibitors. **G. Zhang**

BIOL **238.** Relationship between metal binding and protein stabilization of an ancestral βγ-crystallin from the *Ciona intestinalis tunicate*. **N. Kozlyuk**, S. Sengupta, J. Bierma, R.W. Martin

BIOL **239.** Using light and a photoactivated insulin depot to control insulin release and blood glucose in-vivo. **B.R. Sarode**, K. Kover, P.Y. Tong, C. Zhang, S.H. Friedman

BIOL **240.** *C9orf72* repeat expansion disrupts nucleocytoplasmic transport. **S. Bifulco**, K. Zhang

BIOL **241.** Development of highly specific carbohydrate-nucleic acid reagents for lectin recognition. **C. Gordon**, J. Niu, A. Pusuluri, A. Csordas, C.J. Hawker, H. Soh

BIOL **242.** Synthesis of solvatochromic probes to study the effect of host microenvironment on mycobacterial cell wall dynamics during infection. **S. Keyser**, A. Utz, C.R. Bertozzi

BIOL **243.** Cryptic antibiotic discovery in the filamentous cyanobacterium Scytonema sp. UTEX LB 1163. **M.L. Hillwig**

BIOL **244.** Chemo-enzymatic synthesis of an effective bifunctional NAADP analog for isolation and purification of the NAADP receptor. **P. Su**, T. Walseth, J. Slama

BIOL **245.** Ribonucleotide reductase enzyme a target for titanium complexes: A strategy to cure cancer. **K. Gaur**, S.C. Perez, E. Akam, E. Tomat, M. Saxena, R.K. Sharma, A.D. Tinoco

BIOL **246.** Inhibition of cancer cell viability and selective inhibition of lysyl oxidase with small-molecule Inhibitors. **K. Johnston**, K.M. Lopez

BIOL **247.** Plausible reaction mechanism of the deamination of histidine catalyzed by histidine-ammonia lyase. **S. Minkowicz**, Y. Sheng

BIOL **248.** Unraveling the role of ligands in the hydrogen evolution mechanism catalyzed by [NiFe] hydrogenases. **S. Qiu**, L.M. Azofra, D.R. MacFarlane, C. Sun

BIOL **249.** Highly responsive and selective fluorescent probes to image ATP in live cells. **Y. Fan**, H. Ai

‡ *Cooperative Cosponsorship*

BIOL **250.** Design of a two-step fluorogenic strategy for tyrosine specific labeling of proteins. **M. Shadmehr**, M. Stagg, J.C. Jewett

BIOL **251.** Development of a direct activity probe for a critical regulator of metastatic signaling. **T. Hamada**, J.R. Beck, G.R. Casey, M. Kelly, X. Zhou, C.I. Stains

BIOL **252.** Spatial and temporal control of lysine acetyl transferases (KATs): Ligand gated split KATs. **C.S. de Silva**

BIOL **253.** Determination of metal affinities of *Halobacterium salinarum* cysteinyl-tRNA synthetase. **L. Cobani**, J. Kuhlmeier, J. Rosentreter, C.M. Evilia

BIOL **254.** Irradiation-controlled disassembly of peptide hydrogels and dye release via photolabile Lys(Nvoc). **J. Pellegrino**, R.M. Abaskharon, F. Gai

BIOL **255.** DNA repair proteins XLF and XRCC4 interact with telomeric proteins TRF1 and RAP1. **P. Zaibaq**, **M. Guirette**, E. Castle, K. Vu, N. Fahmy, J. Jabbur, A. Ribes-Zamora

BIOL **256.** Evolved luciferases improve activity with pyridone luciferins. **B.S. Zhang**, K.A. Jones, D.C. McCutcheon, J.A. Prescher

BIOL **257.** Development of antifungal α/β-peptides mimetics of the antimicrobial peptide Aurein 1.2. **M. Lee**, N. Raman, A. Rodriguez-Lopez, S.H. Gellman, D.M. Lynn, S. Palecek

BIOL **258.** Engineering Modular Polyketide Synthases for Generation "Drop In" Biofuels. **C.B. Bailey**, A. Zargar, R. Anayah, S. Curran, L. Katz, J.D. Keasling

BIOL **259.** Development of *Streptomyces as heterologous* hosts for the production of branched fatty acids for biofuels. **R. Krishna**, **J. Blake-Hedges**, R. Haushalter, J.D. Keasling

BIOL **260.** Synthesis and biochemical assessment of hydroxytyrosol. **I. Kady**, E. Onobun, S. Mumford

BIOL **261.** Proline-rich peptides inhibit polymerization of sickle cell hemoglobin. **B.B. Brennan**, L. Steenberge

BIOL **262.** Investigation of the effect of gold nanoparticles on the structure and catalytic function of *Escherichia coli* prolyl-tRNA synthetases. **S. Mitchell**, **O. Hurst**, A. Lato, J.A. Dahl, S. Hati

BIOL **263.** LGN protein purification for X-ray crystallography. A. Howard, A.H. Smith, R. Elnicki, J. Galardi, L.B. Cook, **B.M. Sreenilayam**

BIOL **264.** Measuring metabolite consumption by *Sinorhizobium meliloti* using 1H NMR spectroscopy and time domain Complete Reduction to Amplitude Frequency Table (CRAFT). **D.P. Soulsby**, D.B. Wacks, N. Stubb

BIOL **265.** Development of a cannabinoid-based Cell-in-a Box® therapeutic system targeted toward malignant tumors. R.M. Hyslop, **C.E. Brown**, A. Magiotta, B. Morgan, M. Brown, T. Sherman, D. Petty, S. Desa, J. O'Neil, S. Flora, K. Kellogg, C. Hansen, S. Bydalek, T. Cale, C. Laster, J. Folsom, A. Hawkinson

BIOL **266.** Cartilage: Function and supramolecular structure. **F. Horkay**, E.K. Dimitriadis, I. Horkayne-Szakaly, P.J. Basser

BIOL **267.** Photosensitized oxidation of biotinylated dyes. **R.A. Haack**, Q. Ruan, K.M. Swift, S. Tetin

BIOL **268.** Purification of a putative tartrate-resistant acid phosphatase from *Penicillium spinulosum*. B.A. Schofield, J. Carsella, **S.J. Bonetti**

BIOL **269.** Evaluation of potential functions of two previously uncharacterized bacterial GNAT threonine N-acetyltransferases from *Clostridium difficile and Staphylococcus aureus*. J. Baumgartner, D. Tran, **M.L. Kuhn**

BIOL **270.** Discovery of endogenous and synthetic ligands for orphan nuclear receptor TLX. **A.C. Cao**, P. Kandel, M. Maletic-Savatic, D. Young

BIOL **271.** Synthesis, characterization and biological studies of cobalt(II) Schiff bases derived from *o-vanillin* with series of aromatic amines. **R.O. Shaibu**

BIOL **272.** Spectroscopic and computational studies on the comparative interaction of cationic single-chain and gemini surfactants with hen egg white lysozyme. **R. Patel**

BIOL **273.** Evaluating Fmoc-amino acids as butyrylcholinesterase inhibitors. **J.P. Schwans**, J. Ramirez, J. Gonzalez

BIOL **274.** -2-Himachalen-6-ol: A novel anticancer sesquiterpene unique to the Lebanese wild carrot. **R.I. Taleb**, C. Daher, M. Mroueh, M. ElSibai

BIOL **275.** Reverse transport of 1-Methyl-4-Phenylpyridirum (MPP+) is mediated by extracellular calcium in dopaminergic MN9D cells. **V.Q. Le**, K. Wimalasena, S. Mapa

BIOL **276.** Glycoconjugated site-selective DNA-methylating agent targeting glucose transporters on glioma cells. M. Buchanan, N. Chase, N. Neill, M. White, C. Kelly, K. Mastro-Kishton, L. Chauvigne-Hines, T. Goodwin, A. McIver, L.J. Bartolotti, A. Bourdelais, A. Frampton, **S. Varadarajan**

BIOL **277.** Disabling WTA to kill MRSA with beta-lactam antibiotics. **C.V. Rice**, M. Foxley, M. Xiao, S. Wright, S. Strange

BIOL **278.** Heteromultivalency in melanoma with GPCR ligands: Target validation and use of orthogonal chemistries towards a heterobivalent scaffold. **J.A. Rodriguez Corrales**, D.H. Clark, P. Kohnke, J.S. Josan

BIOL **279.** NitroTyrosine: Gain-of-function alterations to calcium signaling. **J. Porter**, R.A. Mehl

BIOL **280.** Traversing the challenges of extended conjugation: Bacteriochlorins and aza-bodipys, a new era in photomedicine. **M. Cheng**, R.W. Boyle

BIOL **281.** Bioelectrochemical detection of endocrine disrupting compounds. **A.L. Furst**, A. Hoepker, M.B. Francis

BIOL **282.** Cytochrome c-induced permeabilization of cardiolipin-containing phospholipid membranes is induced through the selective interaction of cytochrome c with cardiolipin. **J.P. Kitt**, D.A. Bryce, S.D. Minteer, J.M. Harris

BIOL **283.** Correlation between melatonin and cortisol levels in hair and their validity as biomarkers. **A. Alarbi**, W. Potter

BIOL **284.** Propargyl-linked antifolates potently inhibit US clinical *S. aureus* isolates with newly identified dfrG and dfrK resistance genes. **S.M. Reeve**, A.C. Anderson, D. Wright

BIOL **285.** Development and application of novel small molecule calcium sensors for investigating neuronal activity. **A.A. Contractor**

BIOL **286.** Engineering alternative radical rebound chemistry the αKG oxygenase Factor Inhibiting Hypoxia Inducible Factor (FIH). **V.D. Chaplin**, M. Knapp

BIOL **287.** Withdrawn.

BIOL **288.** Determination of calreticulin-ligand complex formation using fluorescence sprectroscopy. **C. Thomas**

BIOL **289.** Isomerically pure tetramethylrhodamine voltage reporters. **P. Deal**, E. Miller

BIOL **290.** Design and application of new voltage sensitive dyes for *Ex vivo* brain imaging. **R. Kulkarni**, E. Miller

BIOL **291.** Withdrawn.

BIOL **292.** Investigating active site dynamics in a thermophilic enzyme through FTIR and 2DIR spectroscopy. **T.D. Hill**, H.H. Lepird, D.A. Price, S.D. Moran

BIOL **293.** Dynamics of thrombin generation and flux from clots during whole human blood flow over collagen/tissue factor surfaces. **S. Zhu**, Y. Lu, T. Sinno, S. Diamond

BIOL **294.** Internally quenched synthetic peptides for the study of yeast Ste24p proteolytic activity. **E.A. Krautkramer**, E. Hsu, C. Hrycyna, M.D. Distefano

BIOL **295.** Tissue-specific ascaroside production in the nematode *Caenorhabditis elegans*. **A.E. Akagi**, P. Sternberg, F. Schroeder

BIOL **296.** Stable-on-the-table enzymes: Interlocking of laccase in Whatman filter paper. **C. Riccardi**, C.V. Kumar, R. Kasi

BIOL **297.** Synthetic foldamers as inhibitors of Aβ aggregation. **S. Kumar**, A. Hamilton

BIOL **298.** Characterization of cold adaptation in Antarctic toothfish eye lens proteins. **J. Bierma**

BIOL **299.** Host cell entry of Zika virus may be mediated by glycosaminoglycans. **S.Y. Kim**, J. Zhao, X. Liu, L. Lin, X. Zhang, F. Zhang, R.J. Linhardt

BIOL **300.** Fibrinogen αC (233-425): A model protein for characterizing cross-linking by the transglutaminase factor XIII. **K. Mouapi**, J. Bell, K. Smith, R. Ariens, H. Philippou, M.C. Maurer

BIOL **301.** Withdrawn.

BIOL **302.** Ionic interactions of collagen and thermosetting resin composites. **A. Lorts**, A. Stewart, R. Quirino

BIOL **303.** Characterizing the atypical protein kinase 9 in *Plasmodium*. **A. Eubanks**, R. Raphemot, E. Derbyshire

BIOL **304.** Withdrawn.

BIOL **305.** Investigating the ability of small molecule gibberellins to inhibit the NF-kB pathway. **J. Anand**, A.R. Henderson, A.K. Mapp, A.N. Koehler, C. Schindler

BIOL **306.** On the mechanism of slowing down cancer cell migration in the gold nanoparticles treatment. **Y. Wu**, M.R. Ali, M.A. El-Sayed

BIOL **307.** Purification and kinetic assays of recombinant AaCHYMO from the *Aedes aegypti* female mosquito. **O.E. Burata**, A. Rascon

BIOL **308.** Characterizing the genetic fitness landscape of virus-like particles. **E. Hartman**, C. Jakobson, D.T. Ercek, M.B. Francis

BIOL **309.** Mechanistic studies in Flavin Dependent Thymidylate Synthase (FDTS). **K.U. Karunaratne**, M. LeFebvre, J. Villalobos, A. Kohen

BIOL **310.** Insight into the mechanism of a bifunctional diguanylate cyclase enzyme in *Agrobacterium vitis*: A catalytic loop 6, nitric oxide signaling and bacterial biofilm formation. **D. Williams**, N.M. Nesbitt, E.M. Boon

BIOL **311.** Investigation of oligomeric assemblies within the claudin tight junction protein family: A combined computational and experimental approach. **D. Shastry**, F.J. Irudayanathan, S. Nangia, P. Karande

BIOL **312.** Design, synthesis, and conformational analysis of proposed β-turn mimics from isoxazoline-cyclopentane aminols. M. Memeo, M. Mella, **V. Montagna**, P. Quadrelli

BIOL **313.** Design and synthesis of lysine-56 targeting covalent inhibitors of HSP72. **J. Pettinger**, M. Cheeseman, Y. Le Bihan, M. Widya, R.L. van Montfort, K. Jones

BIOL **314.** Exploiting the peptide-binding site to design inhibitors of the KDM4 subfamily. **J. Maw**, Y. Le Bihan, N. Mok, K. Boxall, A. Tumber, V. Bavetsias, J. Blagg

BIOL **315.** Repurposing an aminomutase from *Taxus* plants: Enzymatic conversion of cinnamate epoxides into ring-opened, chiral phenylserines. **P.K. Shee**, N. Ratnayake, O. Goethe, E.E. Onyeozili, K.D. Walker

BIOL **316.** Branched polyethylenimine disables teichoic acid function leading to altered morphologies of Gram-positive bacteria. **M. Foxley**, S. Wright, M. Xiao, S. Strange, C.V. Rice

BIOL **317.** Protein power: Enzyme-hydrogels for efficient sugar-to-power conversion in a biofuel cell. **A. Ghimire**, A. Pattammattel, R. Kasi, C.V. Kumar

BIOL **318.** Protein phosphor materials: A new generation of biodegradable, multi-functional, protein-based, hydrogels for white emission, sensing of small molecules, and detection of pH over a wide range (3-11). **K.R. Benson**, A. Ghimire, R. Kasi, C.V. Kumar

BIOL **319.** Inhibition of fibrillar assemblies of l-phenylalanine by crown ethers: A potential approach toward phenylketonuria. **D. Banik**

BIOL **320.** Assay interference and off-target liabilities of reported histone acetyltransferase inhibitors. **J.L. Dahlin**, K.M. Nelson, J.M. Strasser, D. Barsyte-Lovejoy, J.H. Shrimp, J.L. Meier, C.H. Arrowsmith, P. Brown, J.B. Baell, M.A. Walters

BIOL **321.** Epigenetics and *O*-GlcNAc cycling: The relationship between dynamic *O*-linked glycosylation and transcriptional regulation. **K.R. Harwood**, J. Hanover

BIOL **322.** Withdrawn.

BIOL **323.** Enzymatically self-assembled functional RNA nanostructures and their therapeutic applications. **H. Kim**, J. Lee

BIOL **324.** Withdrawn.

BIOL **325.** Withdrawn.

WEDNESDAY MORNING

Section A

Moscone Center

131

Self-Assembly of Small Molecules in the Cellular Milieu

B. Xu, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 BIOL **326.** Molecular prosthetics for missing ion transport proteins. **M.D. Burke**

9:10 BIOL **327.** Protein responsive supramolecular assembly for live cell imaging. **I. Hamachi**

9:45 BIOL **328.** Enzyme-instructed self-assembly in cellular milieu: Bioinspired targeting of cancer cells without drug resistance. H. Wang, Z. Feng, J. Zhou, X. Du, **B. Xu**

10:20 Intermission.

10:35 BIOL **329.** Self-assembly of chemotherapeutic colloidal drug aggregates. **M.S. Shoichet**, A. Ganesh, C. McLaughlin, J. Logie, S.C. Owen, B. Shoichet

11:10 BIOL **330.** Mechanism of cell death induced by a small-molecule forming fibrils. **O. Julien**, J.A. Wells

Section B

Moscone Center

132

Mid-Career Investigators in Biological Chemistry

L. Hedstrom, *Organizer*

C. I. Stains, *Presiding*

8:30 Introductory Remarks.

8:35 BIOL **331.** Nanobody activation immunotherapeutics. **B. McNaughton**

8:55 BIOL **332.** Highly selective and sensitive fluorescent probes for superoxide, peroxynitrite, hypochlorous acid, hydrogen peroxide and hydroxyl radical. J. Hu, N. Wong, T. Peng, X. Bai, M. Lu, S. Ye, **D. Yang**

9:15 BIOL **333.** Allosteric modulation of G protein coupled receptors: The P2Y1 receptor as an example. **Z. Gao**, K.A. Jacobson

9:35 BIOL **334.** Role of intrinsic dynamics on substrate binding and catalysis of Escherichia coli prolyl-tRNA synthetase. **S. Hati**

9:55 Intermission.

10:05 BIOL **335.** Chemical probes for the investigation of natural product assembly: Biosynthetic insights and novel opportunities. **M. Tosin**, C. Ho, I. Wilkening, E. Riva, J. Havemann

10:25 BIOL **336.** Targeting RNA with branched peptide boronic acids: Unnatural amino acids, molecular recognition, and in vitro activity against HIV-1 RRE RNA. **W.L. Santos**, Y. Dai, J. Wynn, A. Peralta, D. Rekosh, M. Hammarskjold

10:45 BIOL **337.** Chemical biology tools to study protin-protein iteractions of the fatty acid synthase – updates from the interface. **M.D. Burkart**

Chemical Biology: Enabling Drug Discovery

Sponsored by ORGN, Cosponsored by BIOL

WEDNESDAY AFTERNOON

Section A

Moscone Center

131

Chemical Probes for Bacterial Imaging

Cosponsored by WCC

E. E. Carlson, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 BIOL **338.** Chemical technologies for illuminating Mycobacterium tuberculosis. **K.E. Beatty**

2:50 BIOL **339.** Probing the dynamics of peptidoglycan biosynthesis with Fluorescent D-amino Acids (FDAAs). **M. Van Nieuwenhze**

3:35 Intermission.

3:50 BIOL **340.** Activity-Based probes for selective imaging of an essential PBP in Streptococcus pneumoniae. **E.E. Carlson**

4:35 BIOL **341.** Chemical insights into methicillin-resistant Staphylococcus aureus. **S. Walker**

5:20 Concluding Remarks.

Section B

Moscone Center

132

Graduate Student & Postdoctoral Fellow Symposium

L. Hedstrom, *Organizer*

W. L. Santos, *Presiding*

2:00 Introductory Remarks.

2:05 BIOL **342.** Utilizing selenocysteine for expressed protein ligation and bioconjugations. **J. Liu**, Q. Chen, S. Rozovsky

2:20 BIOL **343.** Genetic targeting of small molecule voltage indicators using SpyTag/SpyCatcher. **V. Grenier**, E. Miller

2:35 BIOL **344.** Translating unnatural amino acids with phenotypically-diverse computationally-engineered EF-Tu variants. **V. Cox**, E. Gaucher

2:50 BIOL **345.** Constructing de novo small molecules responses via signal-induced protein proximity in mammalian cells: Chemically engineer cell behaviors & signaling. **G. Zeng**, W. Xuan, H. Li, R. Zhang, Y. Wei, L. Breden, F. Liang, W. Wang

3:05 BIOL **346.** Direct proximity tagging of small molecule proteins targets. **Z.B. Hill**, S.B. Pollock, M. Zhuang, J.A. Wells

3:20 Intermission.

3:35 BIOL **347.** Development of novel far-red to near-infrared fluorophores for chemical biology. **X. Zhou**, L. Leisak, R. Lai, J.R. Beck, J. Zhao, C. Elowsky, H. Li, C.I. Stains

3:50 BIOL **348.** Probing innate immunity with tunable synthetic glycopeptides. **M. Zhou**, C. Delaveris, J. Kramer, C.R. Bertozzi

4:05 BIOL **349.** Monitoring thioredoxin redox in live cells with a genetically encoded red fluorescent protein biosensor. **Y. Fan**, H. Ai, M. Makar

4:20 BIOL **350.** SAMDI Mass spectrometry assay for the high-throughput profiling of protein interaction domains with peptide ligands and its application to chromodomains. **P.T. O'Kane**, M. Mrksich

4:50 BIOL **351.** Generation of allosteric chaperones for Glucose-6-Phosphate Dehydrogenase (G6PD) deficiency. **S. Hwang**

THURSDAY MORNING

Section A

Moscone Center

131

Graduate Student & Postdoctoral Fellow Symposium

L. Hedstrom, *Organizer*

M. L. Kuhn, *Presiding*

8:30 Introductory Remarks.

8:35 BIOL **352.** Exploring vectorial chain translocation in assembly line polyketide synthases. **M. Ostrowski**, C. Khosla

8:50 BIOL **353.** What machinery controls the release of peptide mimetics from endosomes? A genome-wide analysis. **A. Steinauer**, J.R. LaRochelle, R.F. Wissner, A. Schepartz

9:05 BIOL **354.** Influenza hemagglutinin fusion domain by advanced NMR using novel orthagonal refinement and BICS curvature measurements. **S.T. Smrt**, A. Draney, J. Lorieau

9:20 BIOL **355.** Discovery of a bacterial gene in the gut microbiome encoding metabolism of dietary lignans. **E. Bess**, J. Bisanz, P. Spanogiannopoulos, E. Waligurski, P. Turnbaugh

9:35 BIOL **356.** Targeting phospholipase A2 to diminish inflammation by developing novel inhibitors. **V. Mouchlis**, **J. McCammon**, **E.A. Dennis**

9:50 BIOL **357.** Investigating the Regiospecificity of an Unusual Bacterial Acyl-CoA Dehydrogenase. **J. Blake-Hedges**, J. Pereira, J. Chen, P.D. Adams, J.D. Keasling

10:05 Intermission.

10:20 BIOL **358.** Characterization of a drug-inactivating enzyme from a prominent human gut microbe. **N. Koppel**, J. Bisanz, P. Turnbaugh, E.P. Balskus

10:35 BIOL **359.** Investigating the molecular basis of algal-bacterial symbioses. **R. Wang**, M. Wilson, M. Seyedsayamdost

10:50 BIOL **360.** Engineering protein structure and small molecule transport of the bacterial microcompartment. **M. Slininger Lee**, C. Jakobson, D.T. Ercek

11:05 BIOL **361.** Structural insight from activity: Functional screening of the entire Arabidopsis GT1 family enables cheminformatic-bioinformatic predictions of glycosyltransferase reactions and protein features. **C. Fehl**, M. Yang, K.V. Lees, E. Lim, W. Offen, G.J. Davies, D. Bowles, S.J. Roberts, B.G. Davis

11:20 BIOL **362.** Enzymatic mechanisms for decorating phenazine antibiotics from Lysobacter antibioticus. **J. Jiang**, Y. Zhao, S. Wright, L. Du

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

BMGT

Division of Business Development and Management

J. Bryant, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Entrepreneurial Opportunities in Chemistry (see *YCC,* Sun)

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions (see *CHAL,* Sun)

The Use of Scientific Information in IP-Related Matters (see *CHAL*, Mon)

BUSINESS MEETINGS:

Business Meeting, 1:00 PM: Sun

SUNDAY AFTERNOON

Section A

Hotel Nikko San Francisco

Carmel I

Chemical Angel Network: Chemists Investing in Chemical Companies

Cosponsored by PROF‡ and SCHB‡
Financially supported by CIEC

J. L. Bryant, M. Vreeke, *Organizers*

S. S. White, *Presiding*

1:30 Introductory Remarks.

1:35 BMGT **1.** News and updates from the Chemical Angel Network (CaN) and its 5th year of supporting chemists and company and job creation. **M. Vreeke**

2:00 Company Presentations.

3:00 Investment Discussion.

3:30 Open Forum.

4:00 Concluding Remarks.

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

SUNDAY EVENING

Entrepreneurial Opportunities in Chemistry

Sponsored by YCC, Cosponsored by BMGT, PROF and SCHB

MONDAY MORNING

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

MONDAY AFTERNOON

Chemical Innovation Partnerships: Industry-University Success Stories

Sponsored by COMSCI, Cosponsored by BMGT

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC‡, PRES‡ and PROF‡

TUESDAY MORNING

Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators

Sponsored by PROF, Cosponsored by BMGT, CHED and PRES

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Materials Chemistry of Solutions & Solids for a Sustainable Future

Sponsored by INOR, Cosponsored by BMGT‡, MPPG and PROF‡

TUESDAY AFTERNOON

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Chemists Leading the Charge: Chemists Using Business Acumen & Transformative Research to Address Societal Needs

Sponsored by INOR, Cosponsored by BMGT‡, MPPG, PRES and PROF‡

WEDNESDAY MORNING

Looking Beyond Your Current Boundaries: What's the Next Step?

Academic Route: PhD to Postdoc to Ass. Prof.

Sponsored by PROF, Cosponsored by BMGT and YCC

WEDNESDAY AFTERNOON

Looking Beyond Your Current Boundaries: What's the Next Step?

Industrial Route: PhD, Postdoc, Scientist

Sponsored by PROF, Cosponsored by BMGT and YCC

CARB

Division of Carbohydrate Chemistry

N. Snyder, *Program Chair*

SUNDAY MORNING

Section A

Grand Hyatt San Francisco
Grand Ballroom East

Wolfrom Award

E. Rozners, N. L. Snyder, *Organizers*

L. Wang, *Presiding*

9:00 Introductory Remarks.

9:10 CARB **1.** Stereoselective synthesis of the legionaminic and pseudaminic acids and their glycosides. B. Dhakal, O. Popik, **D. Crich**

9:40 CARB **2.** New type of fully synthetic self-adjuvanting glycoconjugate vaccines. **Z. Guo**

10:10 CARB **3.** Fighting cancer with a sweet bullet: The development of carbohydrate based anticancer vaccines. **X. Huang**

10:40 Concluding Remarks.

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Drug Delivery

Sponsored by CELL, Cosponsored by CARB

Cellulose Structure & Biosynthesis

In the Plant Cell Wall

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

SUNDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Grand Ballroom East

Isbell Award

E. Rozners, N. L. Snyder, *Organizers*

L. Wang, *Presiding*

1:25 Introductory Remarks.

1:35 CARB **4.** Stabilizing Nod2, an innate immune receptor of bacterial cell wall fragments, in Crohn's disease. **C.L. Grimes**

2:05 CARB **5.** Glycoconjugates constructed on peptoid scaffolds. **K. Kirshenbaum**, R.N. Zuckermann

2:35 CARB **6.** Decoding structure-function relationships in the glycome. **L.K. Mahal**

3:05 Concluding Remarks.

Section A

Grand Hyatt San Francisco
Grand Ballroom East

Gin New Investigator Award

E. Rozners, N. L. Snyder, *Organizers*

L. Wang, *Presiding*

3:20 Introductory Remarks.

3:30 CARB **7.** In vitro evolution of carbohydrate clusters for vaccine design. **I.J. Krauss**

4:00 CARB **8.** Synthesis of heparan sulfate oligosaccharides and glycopeptides. **X. Huang**, W. Yang, S.B. Dulaney, Y. Xu, P. Wang, B. Yang, K. Yoshida, J. Liu

4:30 CARB **9.** Study and application of protein glycosylation. **Z. Tan**

5:00 Concluding Remarks.

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Tissue Engineering

Sponsored by CELL, Cosponsored by CARB

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

Cellulose Structure & Biosynthesis

Evolution of Synthases & Fine Structure of Microfibrils

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

MONDAY MORNING

Section A

Grand Hyatt San Francisco
Grand Ballroom East

Hudson Award

E. Rozners, N. L. Snyder, *Organizers*

L. Wang, *Presiding*

9:00 Introductory Remarks.

9:10 CARB **10.** De Novo Synthesis of oligosaccharide via bi-metallic catalysis. **G.A. O'Doherty**

9:40 CARB **11.** Synthesis and biological evaluation of STn-PS A1 as a tumor immunogen. **P.R. Andreana**

10:10 CARB **12.** Towards rules for carbohydrate synthesis: Insights from computational chemistry. **N.L. Pohl**

10:40 CARB **13.** Synthesis of designer polysaccharides as probes of glycan assembly. **T.L. Lowary**

11:10 CARB **14.** Acetals, ion pairs, and oxocarbenium ions. **D. Crich**

11:40 Concluding Remarks.

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Structure

Sponsored by CELL, Cosponsored by CARB

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Cellulose Structure & Biosynthesis

Mechanism of Synthesis

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Functional Lignocellulosics & Nanotechnology

Tuning Interfacial Phenomena with Ligno-Nanocellulosic Materials

Sponsored by CELL, Cosponsored by CARB and COLL

MONDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Grand Ballroom East

Carbohydrate-Based Hybrid Materials for Nanomedicine

Cosponsored by CELL

R. Narain, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CARB **15.** Glycopolymer monolith for protein separation. **Y. Miura**

2:05 CARB **16.** Genome editing *in vivo* with the delivery of Cas9 ribonucleoprotein and donor DNA complexed to nanoparticles. **N. Murthy**

2:35 CARB **17.** Polymer with trehalose side chains enhances the stability and *in vivo* plasma lifetime of insulin. **K. Mansfield**, Y. Liu, J. Lee, J. Ko, H.D. Maynard

2:55 CARB **18.** Glycocalyx-mimetic interfaces: Sugar-coating the answers to virus binding. **R. Kumar**, D. Krazter, K. Cheng, I. Kopyeva, J. Lahann

3:15 Intermission.

3:30 CARB **19.** Chitosan-based graft copolymers for tissue engineering applications. M. Kaliva, A. Georgopoulou, E. Mygdali, M. Chatzinikolaidou, **M. Vamvakaki**

4:00 CARB **20.** Carbohydrate based nanotheranostics for the management of hypoxic tumors. **R. Narain**

4:30 CARB **21.** Zwitterionic-/glycol-polymers coated polystyrene microspheres as surrogates for studying the interactions between *Cryptosporidium* oocysts and silica surface. **L. Liu**, Y. Wang, R. Narain, Y. Liu

5:00 CARB **22.** Influenza-binding sialylated nanoparticles by combination of RAFT polymerization, reductive amination and gold-thiol self-assembly. B. De Geest

5:20 Concluding Remarks.

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Structure

Sponsored by CELL, Cosponsored by CARB

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

Lignin Conversion & Upgrading

Sponsored by CATL, Cosponsored by CARB and ENFL

Cellulose Structure & Biosynthesis

Synthase Trafficking & Synthesis of plant (1->3),(1->4)-D-glucans

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Functional Lignocellulosics & Nanotechnology

Modification & Analytics

Sponsored by CELL, Cosponsored by CARB and COLL

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

N. L. Snyder, *Organizer*

8:00 - 10:00

21. See previous listings.

38-42, 46-47, 50, 53, 57-58, 60-61, 67, 72, 75, 77, 79-80. See subsequent listings.

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TUESDAY MORNING

Section A

Grand Hyatt San Francisco
Grand Ballroom East

LPS: Chemistry, Synthesis & Applications

Cosponsored by CELL

P. G. Wang, *Organizer*

D. E. Kahne, *Presiding*

8:30 Introductory Remarks.

8:35 CARB **23.** Polymerases, terminators, molecular rulers and transporters – integrated quality control systems for establishing the chain length of LPS O antigens. **C. Whitfield**

9:05 Discussion.

9:15 CARB **24.** Using the LPS biosynthetic enzyme heptosyltansferase I to explore protein dynamics of a GT-B glycosyltrasferase. **E.A. Taylor**

9:45 Discussion.

9:55 CARB **25.** Discovery of a novel Wzz3 co-polymerase protein in *Pseudomonas aeruginosa* via data-mining of whole genome sequences. **J. Lam**

10:25 Discussion.

10:35 CARB **26.** Withdrawn.

11:05 Discussion.

11:15 CARB **27.** Studies on the assembly of the outer membrane in E. coli. **D.E. Kahne**

11:45 Discussion.

11:55 Concluding Remarks.

Section B

Grand Hyatt San Francisco
Grand Ballroom West

Carbohydrate-Based Hybrid Materials for Nanomedicine

Cosponsored by CELL

R. Narain, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CARB **28.** Glycopolymers with selectivity as well as avidity through macromolecular enginnering. **M.I. Gibson**

9:05 CARB **29.** Synthetic glycopolymers for recognizing cells and bacteria. **G. Chen**

9:35 CARB **30.** Broad-spectrum and highly selective antiviral macromolecular assemblies that mitigate resistance. **M. Fevre**, Y. Yang, J. Hedrick

9:55 Intermission.

10:10 CARB **31.** Trehalose-grafted glycopolymers and glyconanomaterials for the detection and drug delivery to mycobacteria. **M. Yan**

10:40 CARB **32.** Availability of N-quaternized groups determines the bactericide activity of N,N,N-trimethyl chitosan salts. **H.D. Follmann**, T.M. Nobre, O.N. Oliveira

11:00 CARB **33.** Thermo-responsive poly(N-isopropylacrylamide) and cellulose nanocrystals hybrid hydrogels for wound dressing. **P. Singhsa**, K. Zubik, Y. Wang, H. Manuspiya, R. Narain

11:20 Concluding Remarks.

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Novel Derivatives for Demanding Applications

Sponsored by CELL, Cosponsored by CARB

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

Carbohydrate Processing & Upgrading of Biomass-Derived Molecules

Sponsored by CATL, Cosponsored by CARB and ENFL

Cellulose Structure & Biosynthesis

Biochemistry & Cellular Biology

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Functional Lignocellulosics & Nanotechnology

Tuning Interfacial Phenomena with Ligno-Nanocellulosic Materials

Sponsored by CELL, Cosponsored by CARB and COLL

TUESDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Grand Ballroom East

LPS: Chemistry, Synthesis & Applications

Cosponsored by CELL

P. G. Wang, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CARB **34.** Differential induction of innate immune responses by synthetic lipid A derivatives. **G. Boons**

2:05 Discussion.

2:15 CARB **35.** Chemical synthesis of homogeneous and structurally defined bacterial polysaccharide repeating units and their oligomers. **Z. Guo**

2:45 Discussion.

2:55 CARB **36.** New tools for the elucidation of complex polysaccharide biosynthesis pathways. **J.M. Troutman**

3:25 Discussion.

3:35 CARB **37.** Chemical biology approach to explore biosynthesis and biogenesis of lipopolysaccharides. **P.G. Wang**

4:05 Discussion.

4:15 Concluding Remarks.

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Novel Derivatives for Demanding Applications

Sponsored by CELL, Cosponsored by CARB

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

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Advances in Polysaccharides: Practice & Applications

New Developments in the Industrial Sector

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Functional Lignocellulosics & Nanotechnology

Dispersions, Gels, Foams, Colloids & Films

Sponsored by CELL, Cosponsored by CARB and COLL

TUESDAY EVENING

Section A

Moscone Center
Hall D

General Posters

N. L. Snyder, *Organizer*

7:30 - 9:30

CARB **38.** Glycoprotein monosaccharide analysis using HPAE-PAD. **S. Patil**, J. Rohrer

CARB **39.** Development of an alkyne-based therapeutic to covalently target bacterial pathogens based on their distinctive glycans. **R. Herman**, D.H. Dube

CARB **40.** Discovery of genes required for glycoprotein biosynthesis in the gastric pathogen *Helicobacter pylori*. K. Moulton, **D.H. Dube**

CARB **41.** Synthesis of C-4 modified sialic acid 2,3 dehydroderivatives. **M. Lohman**, C. De Meo

CARB **42.** Synthesis of 7-O-substituted derivatives of N-acetyl neuraminic acid. **M. Shadrick**, C. Yu, C. De Meo

CARB **43.** Synthesis of a C-5 thioamide sialyl donor. **B. Jones**, **C. De Meo**

CARB **44.** Effects of picoloyl at C-7 in siaylation reactions. **S. Escopy**, C. De Meo

CARB **45.** Progress towards the synthesis of galactosaminoglycan mimetics for diagnostic and therapeutic applications. **D.J. Akrobetu**, **N.L. Snyder**

CARB **46.** Synthesis of carbohydrate-functionalized oligoproline analogs for multivalent carbohydrate display. **H. Nakanishi**, **N.L. Snyder**

CARB **47.** Synthesis of trehalose-based photosensitizers. **M.A. Burch**, D. Dennis, J.V. Ruppel, **N.L. Snyder**

CARB **48.** SEM-EDS study of calcium and copper alginate bead formation. J. Ayarza, Y.P. Coello, **J. Nakamatsu**

CARB **49.** Fluorescent FPP analogs for the study of UPPS specificity. **A. Reid**, J. Troutman

CARB **50.** Development and analysis of a novel targeting strategy for bacterial sugars. **K.M. Erickson**, P.M. Scott, J.M. Troutman

CARB **51.** Replacement of endogenous isoprenoids with fluorescent probes in *Escherichia coli*. **C. George**

CARB **52.** Application of newly developed Karplus equations for C(sp2)-O-C-H dihedral angles to the conformational analysis of ester linked carbohydrate derivatives. **S. Hackbusch**, A. Watson, S. Do, A. Franz

CARB **53.** New Karplus Equations for α-1,6-linked Glycans. **A. Watson**, S. Do, A. Franz

‡ *Cooperative Cosponsorship*

CARB **54.** Diaryliodonium salts as useful tools for metal-free arylation of carbohydrates. **C.M. Braun**, S. Townsend

CARB **55.** Synthesis of and evaluation of boronic acid derived lectin mimetics. **J. Whited**, X. Sun

CARB **56.** Application of TiO2 nanostructure for sustainable removal of moisture from air. S. Ferdousi, **M. Hasan**, K. Yeung

CARB **57.** Mechanochromic properties of cellulosic liquid crystalline materials. **K. Miyagi**, Y. Teramoto

CARB **58.** Preservation of labile biomolecules in cellulose nanofiber pills and their biosensing applications. **R. Murase**, Y. Teramoto

CARB **59.** Synthesis and evaluation of an expanded set of chemical reporters for probing mycoloylation in mycobacteria. **T. Fiolek**, H.W. Kavunja, N. Holmes, B. Swarts

CARB **60.** Synthesis and evaluation of a fluorogenic probe for trehalose dimycolate hydrolase in *Mycobacterium*. **C.N. Ramsey**, B.M. Swarts, H.W. Kavunja, N. Holmes

CARB **61.** Chemoenzymatic synthesis of UDP glucose by reversing the direction of the trehalose synthase TreT. B.M. Swarts, **P. Woodruff**

CARB **62.** Inhibition of mycobacterial growth and biofilm formation by chemoenzymatically synthesized trehalose analogues. **J.M. Wolber**, B. Urbanek, L. Meints, I. Lopez-Casillas, B.M. Swarts, P. Woodruff

CARB **63.** De Novo chemical synthesis of 3-azido-3-deoxy-myo-inositol via Ferrier rearrangement. **K. Bednarz**, B. Swarts

CARB **64.** Investigating the substrate specificity of the trehalose-recycling transporter SugABC-LpqY in Mycobacteria. **M. O'Neill**, Z. Wagar, A. Stothard, L. Meints, S. Rundell, B.M. Swarts

CARB **65.** Withdrawn.

CARB **66.** Deoxfluoro-D-trehalose (FDTre) analogues as potential PET probes for imaging mycobacterial infection. **C. Olson**, S. Rundell, Z. Wagar, L. Meints, M. O'Neill, B. Piligian, A. Poston, R.J. Hood, P. Woodruff, B.M. Swarts

CARB **67.** Chemoenzymatic synthesis of 2-amino-modified trehalose analogues. **J. Groenevelt**, L. Meints, B.M. Swarts

CARB **68.** Exploiting trehalose metabolism to deliver Antibody-Recruiting Small Molecules (ARMs) to mycobacteria. **A. Rylski**, H.W. Kavunja, B.M. Swarts

CARB **69.** Comparison of microwave-mediated sugar linker reactions. **D. Dimas**, K.D. McReynolds

CARB **70.** Synthesis of a novel glycodendrimer through green and sustainable methods. **C. Vierra**, K.D. McReynolds

CARB **71.** Synthesis and fluorescent labeling of lacto-*N*-tetraose. **K. Craft**, S. Townsend

CARB **72.** Tuning hyaluronic acid binding properties to CD44 using synthetic, *in vitro* and *in silico* approaches. **D.S. Bhattacharya**, D. Svechkarev, J. Souchek, T. Hill, M. Taylor, A. Natarajan, A. Mohs

CARB **73.** Genotoxic agents conjugated inhibitors of glucose transporter for anti-colorectal cancer. **C. Chang**, H. Yang, P. Liang

CARB **74.** Design, synthesis and antitumor evaluation of novel 2-amino-2-deoxysugar-bearing pentacyclic triterpenoid saponin derivatives. **Y. Lin**, Y. Juang, P. Liang

CARB **75.** Synthesis and evaluation of cell-permeable analogs of trehalose. **J. Bragg**, M.G. Paulick

CARB **76.** Understanding the biosynthetic transformation of carohydrate metabolic chemical reporters. **A. Batt**, M. Pratt

CARB **77.** Composition, stability and structure of calcium-complex(es) of isosaccharinate forming in hyperalkaline aqueous solutions. **C. Dudas**, B. Kutus, I. Palinko, P. Sipos

CARB **78.** Multinuclear complex formation between Ca(II) and L-gulonate in strongly alkaline medium. **B. Kutus**, G. Peintler, I. Palinko, P. Sipos

CARB **79.** Synthesis of neoglycoproteins for the potential diagnosis and follow-up of leishmaniasis and Chagas disease. **A.L. Montoya**, R.A. Ashmus, K. Michael

CARB **80.** Regioselective trifluoromethylation and pentafluoroethylation of glycals and electron-rich alkenes using Cu(CF2)nCF3 reagents. J. Mestre, O. Boutureira, A. Lishchynsky, V. Grushin, **S. Castillon**

CARB **81.** Micro/nanoparticles prepared from kappa-, iota-, and lambda-carrageenan for versatile use. **N. Sahiner**, S. Sagbas, S. Yilmaz

CARB **82.** Transparent cassava-based cellulose film production using carbon dioxide switchable polarity solvent. P. Nanta, **K. Kasemwong**, W. Skolpap, Y. Shimoyama

WEDNESDAY MORNING

Section A

Grand Hyatt San Francisco
Grand Ballroom East

Carbohydrate-Based Nanomaterials & Drug-Delivery Vehicles

Cosponsored by CELL

Y. C. Lee, W. F. Vann, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CARB **83.** Cell response at the interface of carbohydrates and nanomaterials. J. Du, R. Bhattacharya, **K.J. Yarema**

9:05 CARB **84.** Human influenza virus receptors. **J.C. Paulson**, W. Peng, R.P. de Vries, O.C. Grant, A.J. Thompson, R. McBride, I.A. Wilson, R.J. Woods

9:35 CARB **85.** Glycocluster: Use of multivalent-type carriers for assembly of carbohydrates. **K. Matsuoka**

10:05 CARB **86.** Acid-degradable mannosylated nanogels for dendritic cell targeted immunotherapy. **R. De Coen**, B. De Geest

10:25 Intermission.

10:45 CARB **87.** Systemic clearance: Natural and synthetic glycosaminoglycan-based drugs are cleared by the stabilin family of receptors. **E.N. Harris**

11:15 CARB **88.** Nanostructured glycan architecture is important in the inhibition of influenza A virus infection. S. Kwon, D.H. Na, J.H. Kwak, M. Douaisi, F. Zhang, E.J. Park, J. Park, H. Youn, C. Song, R.S. Kane, J.S. Dordick, K.B. Lee, **R.J. Linhardt**

11:45 CARB **89.** Withdrawn.n

12:05 CARB **90.** Synthesis of novel biodegradable sacharides-containing polymers and nanoparticles with biomedical applications. **K.T. Petrova**

Bio-based Gels & Porous Materials

Biopolymer Hydrogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Polysaccharides: Practice & Applications

Novel Biocatalytic & Biopolymeric Approaches

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Functional Lignocellulosics & Nanotechnology

Dispersions, Gels, Foams, Colloids & Films

Sponsored by CELL, Cosponsored by CARB and COLL

WEDNESDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Grand Ballroom East

Carbohydrate-Based Nanomaterials & Drug-Delivery Vehicles

Cosponsored by CELL

Y. C. Lee, W. F. Vann, *Organizers*, *Presiding*

1:30 CARB **91.** Gene expression mediated by N-glycan targeted DNA nanoparticles. **K. Rice**

2:00 CARB **92.** New glycotechnology platform interfacing chemistry and biology. **S. Nishimura**

2:30 CARB **93.** Sugar-based polymers with bioactivity. **K.E. Uhrich**

3:00 CARB **94.** Beta-glucan for therapeutic functional oligonucleotides: Immunocyte targeting DDS with dectin-1. **K. Sakurai**, N. Fujiwara, S. Mochizuki

3:20 Intermission.

3:40 CARB **95.** Water-Soluble synthetic carbohydrate receptor with non-glucosidic selectivity. **A.B. Braunschweig**

4:00 CARB **96.** Supramolecular biomaterials with multi-scale hierarchical order via synthetic glycopeptide self-assembly. **G. Hudalla**, A. Restuccia

4:20 CARB **97.** Sugar-Grafted Trojan Horse nanocarrier for combating planktonic and biofilm bacteria. **K. Neoh**, M. Li, E. Kang, K. Chua

4:40 CARB **98.** Adhesion of microcomposites based on yeast glucan particles in 3D cell culture perfusion environment. **I. Salon**

5:00 Concluding Remarks.

Bio-based Gels & Porous Materials

Biopolymer Organogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Polysaccharides: Practice & Applications

Novel Materials & Methodologies

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Functional Lignocellulosics & Nanotechnology

Responsive Materials & Biosensors

Sponsored by CELL, Cosponsored by CARB and COLL

Frontiers in Glycoanalytics

MS & NMR Methods

Sponsored by CELL, Cosponsored by ANYL, CARB‡ and MPPG‡

THURSDAY MORNING

Bio-based Gels & Porous Materials

Aero-, Cryo- & Xerogels

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Advances in Polysaccharides: Practice & Applications

New Functional Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Functional Lignocellulosics & Nanotechnology

Responsive Materials & Biosensors

Sponsored by CELL, Cosponsored by CARB and COLL

Frontiers in Glycoanalytics

Molar Mass & Crystallinity Analyses

Sponsored by CELL, Cosponsored by ANYL, CARB‡ and MPPG‡

THURSDAY AFTERNOON

Bio-based Gels & Porous Materials

Open-Porous Carbon Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Polysaccharides: Practice & Applications

Preparation, Characterization & Applications

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Functional Lignocellulosics & Nanotechnology

(nano)Paper: From Fundamentals to Applications/Antimicrobial, Functional Materials

Sponsored by CELL, Cosponsored by CARB and COLL

CATL

Division of Catalysis Science and Technology

E. Nikolla and S. Scott, *Program Chairs*

SUNDAY MORNING

Section A

Parc 55 San Francisco

Mission I

Advanced X-Ray Techniques for Catalyst Characterization

Catalysts in Action

Cosponsored by PHYS

A. M. Karim, *Organizer*

S. R. Bare, *Organizer, Presiding*

8:00 CATL **1.** Multi-modal *operando* investigations of activities and phase transformations of supported Pd nanocatalysts during ethylene hydrogenation reaction. **Y. Li**, S. Zhao, D. Liu, R.G. Nuzzo, E. Stach, A. Frenkel

8:20 CATL **2.** X-ray characterization of subnanometer cluster-based catalysts. **S. Vajda**

8:50 CATL **3.** Application of lab-based AP-XSP to operando studies of catalysis. **F. Tao**

9:20 CATL **4.** Catalysts for selective hydrogenation of furfural derived from [Pd(NH3)4](ReO4)2 on γ-Al2O3: Advanced characterization by EXAFS, STEM-EDX, and complementary techniques. **H. Lamb**, S. Thompson

9:40 Intermission.

10:10 CATL **5.** *Operando* x-ray spectroscopy of a catalytic solid: Towards a molecular movie. **B.M. Weckhuysen**

10:50 CATL **6.** Combining *in situ* characterization techniques to reveal real-time deactivation mechanisms in Fischer-Tropsch synthesis catalysts. **M. Ronning**

11:20 CATL **7.** Withdrawn.

Section B

Parc 55 San Francisco

Cyril Magnin III

Amorphous Catalytic Materials

S. L. Scott, *Organizer*

B. Peters, *Organizer, Presiding*

8:00 CATL **8.** Theoretical studies of the solid-liquid interface of γ-alumina supported catalysts: Impact on impregnation and dried state. **M. Corral Valero**, B. Ngouana-Wakou, P. Raybaud

8:35 CATL **9.** Computational studies of catalytic reactions of metal oxide clusters and metal ions in zeolites. Z. Fang, S. Zhang, **D.A. Dixon**

9:10 CATL **10.** Withdrawn.

9:45 Intermission.

10:05 CATL **11.** Dynamic structures and catalytic properties of platinum nanoparticle in carbon nanotube. **G. Wei**, Z. Liu

10:25 CATL **12.** Ab-initio modeling of Zr(OH)4 in the presence of atmospheric contaminants. **I. Iordanov**, V.M. Bermudez, G.W. Peterson, W.O. Gordon, C.J. Karwacki, R. Balow, D. Barlow, I. Schweigert, J. Lundin, D. Gunlycke, P.E. Pehrsson

10:45 CATL **13.** Computational investigation of Lewis and Brønsted acidity in metal-doped mesoporous silicates. A. Jystad, A. Biancardi, **M. Caricato**

11:05 CATL **14.** Structure and reactivity of porous amorphous catalysts: Insights from molecular modeling. R. Chaudret, S. Schweizer, J. Low, **L. Subramanian**

11:25 CATL **15.** Hydroisomerization of n-hexadecane: Remarkable selectivity of platinum nanoparticles supported on amorphous mesoporous silica post-synthetically modified with aluminum. **K. Sabyrov**, N. Musselwhite, G. Melaet, G.A. Somorjai

Section C

Parc 55 San Francisco

Market Street

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Single Crystal Catalysis

Cosponsored by COLL and WCC

C. Kumar, *Organizer*

R. Madix, *Presiding*

8:00 Introductory Remarks.

8:15 CATL **16.** Competition for active sites in steady state catalytic reactions; importance of weak van der Waals interactions. **R.J. Madix**, S. Karakalos, Y. Xu, A. Tkatchenko, F. Kabeer, W. Chen, E. Kaxiras, C.M. Friend

8:45 CATL **17.** Energetics of adsorbed molecular fragments on Ni(111) and Pt(111) by calorimetry: Understanding differences in catalysis by Ni versus Pt. **C.T. Campbell**, S.J. Carey, W. Zhao

9:15 Intermission.

9:30 CATL **18.** Structure-reactivity relations through charge control at the atomic level in heterogeneous catalysis. **H. Freund**

10:00 CATL **19.** Single atom alloys for efficient and cost-effective catalysis. **E.H. Sykes**

10:30 Intermission.

10:45 CATL **20.** Understanding the catalytic activity of Pt-Re bimetallic surfaces. A.J. Brandt, T.D. Maddumapatabandi, G.S. Seuser, K. Xie, A. Duke, **D.A. Chen**

11:15 CATL **21.** Oxygen surface chemistry for energy conversion processes. **J.K. Norskov**

Section D

Parc 55 San Francisco

Cyril Magnin I

Electrocatalysis for Energy Generation & Storage

Oxygen Reduction

Cosponsored by ENFL

A. Holewinski, C. Wang, H. Xin, *Organizers*

J. Snyder, *Organizer, Presiding*

A. Holewinski, *Presiding*

8:00 CATL **22.** Platinum alloy nanocatalyst with manipulated particle composition and morphology for improved ORR property. **Z. Peng**, C. Zhang, S. Hwang

8:20 CATL **23.** Morphological and compositional instability in nanoporous nanoparticle electrocatalysts for oxygen reduction reaction. **Y. Li**, J. Snyder

8:40 CATL **24.** Enhanced electrocatalysis for polymer electrolyte membrane fuel cells and electrolyzers. **M. Escudero-Escribano**, A.L. Strickler, T.F. Jaramillo, I. Stephens, I. Chorkendorff

9:00 CATL **25.** Phase segregated copper silver thin films as model catalysts for electrochemical oxygen reduction in alkaline electrolytes. **D.C. Higgins**, B. Gibbons, C. Hahn, M. Wette, B. Clemens, T.F. Jaramillo

9:20 Intermission.

9:40 CATL **26.** From well-defined electrochemical interfaces to functional nanoscale materials. **V. Stamenkovic**

10:20 CATL **27.** Withdrawn.

10:40 CATL **28.** Nitrogen-doped Carbon Nanostructures (CNx) as as bifunctional electrocatalysts for oxygen reduction reaction and oxygen evolution reaction in acidic media. K. Mamtani, D. Jain, A. Co, **U.S. Ozkan**

11:00 CATL **29.** Nitrogen doped double gyroidal mesoporous carbon materials for oxygen reduction reaction synthesized from pyridine containing precursor, hydroxymethyl-3-hydroxylpyridine. **F. Matsuoka**, Q. Zhang, U.B. Wiesner

11:20 CATL **30.** Manganese deception on graphene. **R. Ye**, R. MendozaCruz, Y. Li, M.J. Yacaman, J.M. Tour

11:40 CATL **31.** Flexible bifunctional oxygen electrode through morphological emulation of human hair array for rechargeable zinc air batteries. **J. Fu**, F. Hassan, Z. Chen

Section E

Parc 55 San Francisco

Cyril Magnin II

Synthesis of Catalysts by Non-Traditional Methods

Nanoparticle Catalysts

Cosponsored by COLL and INOR

A. Alba-Rubio, T. J. Schwartz, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:10 CATL **32.** Electrostatic adsorption for synthesis and size control of supported metal catalysts. A. Wong, Q. Liu, S. Eskandari, **J.R. Regalbuto**

8:40 CATL **33.** Aerosol synthesis of shape-controlled nanomaterials for photocatalytic applications. **S.E. Skrabalak**

9:10 CATL **34.** Development of a new generation of stable, tunable, and catalytically active nanoparticles produced by the helium nanodroplet deposition method. **A. Orlov**, Q. Wu, J. Cen, C.J. Ridge, M. Lindsay, S. Zhao, D. Zakharov, E. Stach, E. Connors, X. Tong, D. Su

9:30 CATL **35.** Synthesis and compositional control in highly uniform palladium-based bimetallic nanocrystals for catalytic methane activation. **J. Willis**, E.D. Goodman, M. Cargnello

9:50 CATL **36.** Cobalt-copper nanoparticle catalysts for higher alcohols synthesis prepared by water-in-oil microemulsion. **J.L. Snider**, T.F. Jaramillo

10:10 CATL **37.** Colloidal synthesis, characterization, & selective alkyne hydrogenation by supported Ni and Co nanocrystals. **N.S. Dwarica**, J. Bruno, B.D. Chandler, C. Pursell

10:30 CATL **38.** Highly active Au-Pd nanoparticles supported on titanate nanotubes. **M.M. Khawaji**, D. Chadwick

10:50 CATL **39.** Novel Mo/W precursors for supported catalysts with enhanced hydrodesulfurization activity and selectivity. **P. Yuan**

11:10 CATL **40.** Synthesis of catalytic materials by electrospinning with controlled morphology. **M. Guerrero-Perez**, R. Berenguer, I. Guzman, J. Rodriguez-Mirasol, T. Cordero

Section F

Parc 55 San Francisco

Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

Theory

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

8:00 CATL **41.** Catalytic processing of bioethanol on transition state metals. **F. Jalid**, T.S. Khan, M. Haider

8:20 CATL **42.** Withdrawn.

8:40 CATL **43.** Orbital-wise coordination number as a reactivity descriptor for metal nanocatalysts. **H. Xin**, X. Ma, S. Wang

9:20 CATL **44.** Insights into active sites and their environments under working catalytic condition. **M. Neurock**

10:00 CATL **45.** Elucidation of structure and activity using machine learning-accelerated genetic algorithms and kMC. **T. Bligaard**

10:40 CATL **46.** Models and trends in adsorbate-adsorbate interactions at metal surfaces. A. Bajpai, K. Frey, **W.F. Schneider**

11:20 CATL **47.** Modeling segregation in late transition metal alloys across composition space. J. Boes, **J.R. Kitchin**

Synthesis & Characterization of Materials for Energy Applications

Enabling Concepts for Energy Materials Design

Sponsored by ANYL, Cosponsored by CATL

C1 Catalysis

Sponsored by ENFL, Cosponsored by CATL

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Surface Science is Alive & Well

Sponsored by COLL, Cosponsored by CATL

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Catalysis for Unconventional Energy Sources

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Subsurface Technologies for Recovery of Fossil & Geothermal Energy

Sponsored by ENFL, Cosponsored by CATL and GEOC

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

Sustainability in Electrocatalytic Fuel & Chemical Production

Sponsored by INOR, Cosponsored by CATL

SUNDAY AFTERNOON

Section A

Parc 55 San Francisco
Mission I

Advanced X-Ray Techniques for Catalyst Characterization

Theory & Beyond

Cosponsored by PHYS

S. R. Bare, A. M. Karim, *Organizers*

A. M. Karim, *Presiding*

1:00 CATL **48.** Al K-edge XAFS, molecular dynamics-XAFS and the chemistry of zeolite Brønsted acid sites. **J. Fulton**, N. Govind, D. Mei, A. Vjunov, D.M. Camaioni, T. Huthwelker, J.A. Lercher

1:30 CATL **49.** Exploring the anomalous behavior of metal nanocatalysts with finite temperature AIMD and x-ray spectra. **F.D. Vila**, J.J. Rehr, A. Frenkel

2:00 CATL **50.** Environmental sensitivity of spectroscopic properties for Cu ions in Cu-SSZ-13: XANES and XES studies from first principles. R. Zhang, H. Li, K. Groden, F. Gao, J. Szanyi, S.L. Scott, **J. McEwen**

2:30 CATL **51.** Structural characterization of catalysts: Interplay between theory and experiment. **P. Sautet**

3:00 Intermission.

3:30 CATL **52.** Solving dynamic structure of nanoparticles: From model to real catalysts. **A. Frenkel**

4:10 CATL **53.** Crystalline covalent organic frameworks for heterogeneous catalysis. **Y. Zhang**

4:30 Discussion.

Section B

Parc 55 San Francisco
Cyril Magnin III

Amorphous Catalytic Materials

B. Peters, *Organizer*

S. L. Scott, *Organizer, Presiding*

1:00 CATL **54.** Studies of silica- and alumina-supported catalysts by dynamic nuclear polarization solid-state NMR. F.A. Perras, T. Kobayashi, **M. Pruski**

1:35 CATL **55.** Solid state NMR as a powerful tool for the study of alumina-supported organo-metallic catalysts. L. Delevoye, F. Pourpoint, N. Merle, K.C. Szeto, A. Gallo, S.L. Scott, M. Taoufik, **R. Gauvin**

2:10 CATL **56.** Surface Science approach to the Phillips (Cr/SiO2) catalyst. **Q. Pan**, L. Li, S. Shaikhutdinov, H. Freund

2:30 CATL **57.** Well-defined group VI oxo derivatives supported on silica by SOMC: Model of industrial olefin metathesis catalyst. **N. Merle**, Y. Bouhoute, K.C. Szeto, A. De Mallmann, I. Del Rosal, L. Maron, C.P. Nicholas, L. Delevoye, R. Gauvin, M. Taoufik

2:50 Intermission.

3:10 CATL **58.** Spectroscopic properties and coordination environment of silica supported MoO3 catalyst. S. Klepper, Y. Wang, D. Jeffcoat, N. Peek, L.J. Van De Burgt, S.L. Scott, **A.E. Stiegman**

3:45 CATL **59.** Molecular design of cooperative interactions for amorphous silica materials to tune catalytic selectivities. **N.A. Brunelli**, M.R. Whitaker, R. Joshi, A. Parulkar

4:20 CATL **60.** Understanding the role of atmospheric surface adsorbates on the chemical reactivity of zirconium hydroxide nanopowders using *Operando* vibrational spectroscopy. **R. Balow**, W.O. Gordon, D. Barlow, J. Lundin, I.O. Iordanov, C. Knox, V.M. Bermudez, J.H. Wynne, G.W. Peterson, C.J. Karwacki, P.E. Pehrsson

4:40 CATL **61.** Preparation and characterization of amorphous/nanocrystalline thin film catalysts. A. Pfau, S. He, J.T. Diulus, G. Albuquerque, I. Lyubinetsky, **G.S. Herman**

Section C

Parc 55 San Francisco
Market Street

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Single Crystal Catalysis

Cosponsored by COLL and WCC

C. Kumar, *Organizer*

K. J. Stowers, *Presiding*

1:00 CATL **62.** Understanding of atomically-thin materials grown on Au(111). **X. Deng**, D. Sorescu, J. Lee

1:30 CATL **63.** Catalytic C-C bond formation to synthesize carboxylic acids using CO2. **K.J. Stowers**

2:00 Intermission.

2:15 CATL **64.** Adsorption and oxidation reactions on RuO2 and IrO2 surfaces. **J.F. Weaver**, Z. Liang, T. Li, R. Rai, M. Kim, A.R. Asthagiri

2:45 CATL **65.** Recycling of CO2: Probing the chemical state of the Ni(111) surface during methanation reaction. C. Heine, **M. Salmeron**

3:15 Intermission.

3:30 CATL **66.** In-situ liquid phase spectroscopy for characterization and quantification of acid sites in the presence of solvents. **B. Xu**, N. Gould

4:00 CATL **67.** Application of surface science techniques to nanoporous materials: Studies of metal organic frameworks. **L.B. Benz**

Section D

Parc 55 San Francisco
Cyril Magnin I

Electrocatalysis for Energy Generation & Storage

CO_2 Reduction

Cosponsored by ENFL

A. Holewinski, J. Snyder, C. Wang, *Organizers*

H. Xin, *Organizer, Presiding*

A. Holewinski, *Presiding*

1:00 CATL **68.** Mechanistic insights into the electrochemical reduction of CO2 using in-situ surface enhanced spectroscopy. **B. Xu**, M. Dunwell, Q. Lu, J.G. Chen, Y. Yan, F. Jiao

1:20 CATL **69.** Surface structure engineering of Cu thin films for electrochemical CO2 reduction. **C. Hahn**, T. Hatsukade, A. Vailionis, D.C. Higgins, S. Nitopi, T.F. Jaramillo

1:40 CATL **70.** Electrolysis of CO2 to syngas in bipolar membrane-based electrochemical cells. **C.C. Li**, D. Zhou, Z. Yan, R. Gonçalves, D. Salvatore, C.P. Berlinguette, T.E. Mallouk

2:00 CATL **71.** Bimetallic Au-Cu nanocatalysts for enhanced electrochemical CO2 conversion. **D. Kauffman**, D. Alfonso

2:20 CATL **72.** Understanding trends in electrochemical synthesis of fuels and chemicals. **J.K. Norskov**

3:00 CATL **73.** Charge of an ion in the outer Helmholtz plane. **L.D. Chen**, M. Bajdich, C.M. Krauter, J. Martirez, E.A. Carter, A.C. Luntz, K. Chan, J.K. Norskov

3:20 CATL **74.** DFT investigation of CO2 electrochemical reduction to C2 species on copper surfaces: The critical role of surface facet and CO coverage. **P. Hirunsit**, Y. Huang, B.S. Yeo

3:40 CATL **75.** Promoter effects of alkali metal cations during electrocatalytic carbon dioxide reduction. **J. Resasco**, A.T. Bell

4:00 CATL **76.** N-Heterocyclic carbenes as promoters for the heterogeneous reduction of CO2 at metal electrodes. **K.M. Waldie**, C.P. Kubiak

4:20 CATL **77.** Synergistic performance enhancement in graphene nanoribbon – metal nanoparticle composites for electrocatalysis. **C. Rogers**, F.R. Fischer

4:40 CATL **78.** Copper nanoparticle/carbon nanospike catalyst for high-selectivity electrochemical conversion of carbon dioxide. **Y. Song**, **D. Hensley**, A. Rondinone

Section E

Parc 55 San Francisco
Cyril Magnin II

Synthesis of Catalysts by Non-Traditional Methods

Model Catalysts, Microporous Materials & Oxides

Cosponsored by COLL and INOR

A. Alba-Rubio, T. J. Schwartz, *Organizers*, *Presiding*

1:00 CATL **79.** New catalytic structures via atomic layer deposition. **P.C. Stair**

1:30 CATL **80.** Doped Zn-containing magnetic oxides in methanol synthesis: Does the capping polymer matter? N. Baird, J. Dittmar, Y. Losovyj, M. Pink, D.G. Morgan, B. Stein, N. Firsova, E. Serkova, M. Grigoriev, A. Sidorov, M. Sulman, Z. Shifrina, **L. Bronstein**

1:50 CATL **81.** Calixarene-Metal clusters as precatalysts and catalysts. A. To, X. Ouyang, L. Debefve, T. Rea, A. Palermo, B.C. Gates, A. Kuperman, **A.S. Katz**

2:20 CATL **82.** Catalytic consequences of hydrophobic pockets confining Lewis acid sites in beta zeolites for aqueous-phase glucose isomerization. **M.J. Cordon**, J.W. Harris, J. Hall, R. Gounder

2:40 CATL **83.** Ionic liquids for the synthesis of metal aluminophosphate-based catalysts. **S. Citrak**, S.I. Zones, S. Oliver

3:00 CATL **84.** Synthesis of supported metal catalysts using molecular precursors and halide metathesis reactions. **S.L. Scott**

3:30 CATL **85.** Biomineralization and bioinspired synthesis of ceria and transition metal-ceria solid solution nanocrystals. **C.D. Curran**, L. Lu, C.J. Kiely, B. Berger, S. McIntosh

3:50 CATL **86.** Tuning graphitic oxide for initiator - and metal-free aerobic epoxidation of linear alkenes. **S. Pattisson**, E. Nowicka, U. Gupta, G. Shaw, R. Jenkins, D. Morgan, D. Knight, G. Hutchings

4:10 CATL **87.** Withdrawn.

4:30 CATL **88.** Nano-confinement preparations of nano- CuO-MOFs in ceria tubes. **Y. Feng**, J. Feng, J. Jiang, M. Zhang

Section F

Parc 55 San Francisco
Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

1:00 CATL **89.** Selectivity in hydrogenation catalysis: A surface-science study. **F. Zaera**

1:40 CATL **90.** Model systems in heterogeneous catalysis at the atomic scale. **H. Freund**

2:20 CATL **91.** Surface structure and chemistry of a Pd-Cu(111) single-atom alloy from polarization dependent infrared spectroscopy. C.M. Kruppe, J.D. Krooswyk, **M. Trenary**

3:00 CATL **92.** From surface science to practical catalysts for catalytic esterification and acylation. **R.J. Madix**, C.M. Friend, M.L. Personick, B. Xu, L. Wang, B. Zugic, J. Biener, M. Biener

3:40 CATL **93.** Looking at zeolites through the eyes of surface science. **J.A. Boscoboinik**

4:20 CATL **94.** Olefin metathesis by supported WOx/SiO2 catalysts: Structure-Reactivity relationships, number of active sites, and kinetics. S. Lwin, **I.E. Wachs**

4:40 CATL **95.** Interaction of atomic oxygen with Ag(111) and Ag(110) surfaces: Understanding the role of subsurface oxygen in oxidative catalysis by silver. S. Isbill, **S. Roy**

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

C1 Catalysis

Sponsored by ENFL, Cosponsored by CATL

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Catalyst Design

Sponsored by COLL, Cosponsored by CATL

Catalysis for Unconventional Energy Sources

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Sustainability in Electrocatalytic Fuel & Chemical Production

Sponsored by INOR, Cosponsored by CATL

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

SUNDAY EVENING

Sustainability in Electrocatalytic Fuel & Chemical Production

Sponsored by INOR, Cosponsored by CATL

MONDAY MORNING

Section A

Parc 55 San Francisco

Mission I

Advanced X-Ray Techniques for Catalyst Characterization

Electro- & Photo-Catalysis

Cosponsored by PHYS

A. M. Karim, *Organizer*

S. R. Bare, *Organizer, Presiding*

8:00 CATL **96.** Structural kinetics study of redox processes of Pt/C and Pt3Co/C cathode electrocatalysts in a polymer electrolyte fuel cell during an accelerated durability test by in situ time-resolved XAFS. **N. Ishiguro**, S. Kityakarn, O. Sekizawa, T. Uruga, H. Matsui, K. Nagasawa, T. Yokoyama, M. Tada

8:20 CATL **97.** Bismuth-Ionic liquid interface for electrocatalytic CO2 conversion under the lens of x-ray reflectivity. **J. Medina Ramos**, S. Lee, A.A. Hubaud, T.T. Fister, P. Fenter

8:40 CATL **98.** In-operando x-ray spectroscopic insight into biomimetic fuel cell electrocatalyst. **H. Lien**, S. Chang, C. Dong, K. Chen, L. Chen

9:00 Intermission.

9:20 CATL **99.** Withdrawn.

9:40 CATL **100.** *In situ* and *operando* insight into CO2 electroreduction and gas phase hydrogenation catalysts. **B.R. Cuenya**

10:20 CATL **101.** Nano-XAFS imaging of oxygen diffusion in Pt-Ce2Zr2Ox particles during oxygen storage/release. H. Matsui, N. Ishiguro, K. Enomoto, T. Uruga, O. Sekizawa, **M. Tada**

10:40 CATL **102.** Electrochemical carbon deposition from CO2 on nickel and ceria electrodes studied by operando XPS. T. Skafte, Z. Guan, M. Machala, C. Gopal, M. Monti, L. Martinez, E. Stamate, S. Sanna, W. Chueh, **C. Graves**

11:00 CATL **103.** Why is water more reactive than H2 in photocatalytic CO2 conversion into fuels at reaction pressure up to 0.80 MPa? H. Zhang, S. Kawamura, M. Miyano, M. Yoshiba, **Y. Izumi**

11:20 CATL **104.** Evidence for small polaron formation leading to intrinsic photoexcited charge trapping in -Fe2O3. **L.M. Carneiro**, S. Cushing, C. Liu, S.R. Leone

11:40 Discussion.

Section B

Parc 55 San Francisco

Cyril Magnin III

Amorphous Catalytic Materials

B. Peters, S. L. Scott, *Organizers*

N. Brunelli, *Presiding*

8:00 CATL **105.** Cu/ZnO catalysts derived from amorphous zincian georgeite precursors. **G. Hutchings**, S. Kondrat, J. Bartley, S. Taylor, C. Kiely

8:35 CATL **106.** Nanocatalysts based on amorphous porous silica for high-efficient reaction processes. **J. Huang**

9:10 CATL **107.** Ambient temperature NO oxidation over Cr-based amorphous mixed oxide catalysts: Effects from the second oxide components. A. Wang, Y. Guo, C.H. Peden, **F. Gao**

9:30 CATL **108.** Limitations of top-down approaches to synthesize amorphous polymer catalysts for biomass hydrolysis. **M.T. Timko**, M. Emmert, S. Granados Focil, K. Schmidt-Rohr

9:50 Intermission.

10:10 CATL **109.** *In situ* site titration of silica-supported metal oxide catalysts. T.R. Eaton, N.E. Thornburg, S. Ahn, **J.M. Notestein**

10:45 CATL **110.** Two dimensionally dispersed V/SiO2 catalysts for the oxidative dehydrogenation of propane. **I. Hermans**

11:20 CATL **111.** Carbon support effects on the selectivity of Pd/C catalysts for the hydrogenation of multifunctional chemicals. **R.G. Rao**, R. Blume, T.W. Hansen, E. Fuentes, Y.J. Chabal, R. Schloegl, D. Hibbitts, J. Tessonnier

11:40 CATL **112.** Improved graphene oxide sponge as superoleophilic furan coupling catalyst. **S. Dutta**, D.G. Vlachos, B. Saha

Section C

Parc 55 San Francisco

Market Street

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Nanocatalysis

Cosponsored by COLL and WCC

C. Kumar, *Organizer*

M. L. Personick, *Presiding*

8:00 CATL **113.** Metal nanoparticles on metal-oxide nanoparticle supports as model catalysts. **J.C. Hemminger**

8:30 CATL **114.** Nanoporous copper foams as a platform for synthesizing active oxygen reduction and alcohol oxidation catalysts. **A. Co**

9:00 Intermission.

9:15 CATL **115.** Polyhedral metal nanoparticles with bimetallic surfaces: Kinetic control and surface passivation. **M.L. Personick**, M.E. King, H. Jung, A.L. Stone, D.D. Robertson, I.A. Kent

9:45 CATL **116.** Au/TiO2 catalysts for low-temperature oxidation and H2 photoproduction from water. **F. Zaera**

10:15 Intermission.

10:30 CATL **117.** Solar-to-chemical conversion via a standalone photoelectrochemical system. **B. Min**

11:00 CATL **118.** Selectivity in methanol oxidation on Fe2O3 and the effect of Mo dosing. **M. Bowker**, P. Hellier

Section D

Parc 55 San Francisco

Cyril Magnin I

Electrocatalysis for Energy Generation & Storage

Oxygen Evolution

Cosponsored by ENFL

A. Holewinski, J. Snyder, C. Wang, H. Xin, *Organizers*

A. Holewinski, C. Wang, *Presiding*

8:00 CATL **119.** Oxygen evolution with an atomically-precise nickel catalyst. **D. Kauffman**, D. Alfonso

8:20 CATL **120.** Understanding aqueous proton transfer in ruthenium catalyzed water splitting. **N. Govindarajan**, A. Tiwari, B. Ensing, E. Meijer

8:40 CATL **121.** Cobalt modification of Ni-Fe layered double hydroxide and the resulting enhancement for the oxygen evolution reaction. **D.R. Strongin**, A.C. Thenuwara, N. Attanayake, Q. Yan

9:00 CATL **122.** Electrodeposited cobalt oxide catalyst in Fe-spiked KOH electrolyte for efficient evolution of oxygen. **L. Gong**, B.S. Yeo

9:20 Intermission.

9:40 CATL **123.** Design principles of oxides to catalyze oxygen evolution reaction. **Y. Shao-Horn**

10:20 CATL **124.** Near surface alloyed perovskites for catalysis. **L. Zhang**, A. Vojvodic

10:40 CATL **125.** Biotemplated synthesis of NiFe oxide nanocatalysts for oxygen evolution reaction. **C. Li**, W. Zhao

11:00 CATL **126.** Au@MxOy core-shell nanoparticles as catalysts for the oxygen evolution reaction. **A.L. Strickler**, M. Escudero-Escribano, T.F. Jaramillo

11:20 CATL **127.** Improving the HER and OER performance by hydrogenation of electrocatalysts. **X. Chen**

Section E

Parc 55 San Francisco

Cyril Magnin II

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Cosponsored by COLL, ENFL, I&EC and INOR

S. Ardo, G. Dukovic, D. Esposito, I. Sharp, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 CATL **128.** Understanding photoelectrocatalysis from first principles. **E.A. Carter**

8:35 CATL **129.** Resonantly excited photocatalysts and light absorbers for solar fuels. **H. Atwater**

9:05 CATL **130.** Dye sensitized photoelectrosythesis cell: The energy frontier research center for solar fuels and Thomas J. Meyer. **T.J. Meyer**

9:35 Intermission.

9:50 CATL **131.** How to provide solar hydrogen and how to apply it? The activity of artificial photo synthetic chemical process project. **T. Setoyama**

10:20 CATL **132.** CO2 + H2O + sunlight = chemical fuels + O2. **P. Yang**

10:50 CATL **133.** Enhancing photostability of BiVO4 photoanodes for solar water oxidation. **K. Choi**

11:20 CATL **134.** Addressing the fundamental materials challenges in advanced solar-driven water splitting technologies. **E. Miller**

Section F

Parc 55 San Francisco

Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

‡ *Cooperative Cosponsorship*

Surface Science

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

8:00 CATL **135.** Aspartic acid adsorption and decomposition mechanism on Cu surfaces. **A.J. Gellman**, A. Reinicker, Y. Yun, B. Karagoz, S. Dutta

8:20 CATL **136.** Exploring enantioselective hydrogenation on chirally modified surfaces in ultrahigh vacuum. **W.T. Tysoe**

9:00 CATL **137.** Insights into methane activation and oxidation on modified ceria catalysts. J.J. Carey, **M. Nolan**

9:20 CATL **138.** Insight into active sites for methane activation from first principles. Z. Zuo, S. Liu, S. Zhang, J. Rodriguez, **P. Liu**

10:00 CATL **139.** Adsorption and reaction of alcohols on SrTiO3(100) by ambient pressure XPS. **Y. Zhang**, A. Savara, D.R. Mullins

10:20 CATL **140.** Mechanism of CO oxidation on supported Ir and Pt single atoms. Y. Lu, C. Kuo, X. Ma, H. Xin, **A.M. Karim**

11:00 CATL **141.** Alcohols selective aminations: A DFT based micro-kinetics modelling strategy for screening the promising heterogeneous catalysts. **T. Wang**, C. Michel, M. Sabbe, M. Pera-Titus, P. Sautet

11:20 CATL **142.** Alloy catalysis across composition space. **I. Sen**, A.J. Gellman

11:40 CATL **143.** Dynamics, stability, and adsorption states of water on oxidized RuO2(110). **M. Nguyen**, R. Mu, D. Cantu, I. Lyubinetsky, V. Glezakou, R. Rousseau, Z. Dohnalek

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Synthesis & Characterization of Materials for Energy Applications

Enabling Concepts for Energy Materials Design

Sponsored by ANYL, Cosponsored by CATL

C1 Catalysis

Sponsored by ENFL, Cosponsored by CATL

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Soft Interfaces

Sponsored by COLL, Cosponsored by CATL

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Catalysis for Unconventional Energy Sources

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY AFTERNOON

Section A

Parc 55 San Francisco

Mission I

Advanced X-Ray Techniques for Catalyst Characterization

New Methodologies

Cosponsored by PHYS

S. R. Bare, A. M. Karim, *Organizers*

A. M. Karim, *Presiding*

1:00 CATL **144.** Ultra sensitive probing of the local electronic structure based on state-of-the-art Transition-Edge Sensor (TES) technology and soft x-ray spectroscopy. **D. Nordlund**, B.K. Alpert, M.L. Baker, H. Cho, E. Denison, W.B. Doriese, J.W. Fowler, K.J. Gaffney, B. Gao, J. Gard, G. C. Hilton, K.D. Irwin, Y.I. Joe, C. Kenney, J. Knight, T. Kroll, S. Lee, D. Li, R. Marks, M. Minitti, R.A. Mori, H. Ogasawara, G. O'Neil, D. Schmidt, D. Sokaras, D.S. Swetz, Y. Song, C.J. Titus, J. Ullom, T. Weng, C. Williams, B.A. Young

1:20 CATL **145.** Characterizing working catalysts with correlated electron and photon probes. **E. Stach**, Y. Li, S. Zhao, A. Gamalski, D. Zakharov, R. Tappero, J.G. Chen, R.G. Nuzzo, A. Frenkel

1:50 CATL **146.** Applications of x-ray Raman scattering for in-situ material charecterization. **B. Mishra**

2:20 CATL **147.** Metal poisoning of catalyst particles as studied by x-ray imaging at multiple length scales. **F. Meirer**

2:50 Intermission.

3:20 CATL **148.** Piecing together a complete picture of catalysis through operando XRD-PDF-DRIFTS. **K.W. Chapman**

4:00 CATL **149.** Utilizing in-situ small and wide angle x-ray scattering for rapid feedback of nanocrystal catalyst synthesis. **C.J. Tassone**, L. Wu, J. Willis, I. McKay, B. Diroll, M. Cargnello, J. Qin, L. Pellouchoud, A. Fournier

4:30 CATL **150.** Atomic scale strain field distribution of catalyst during the reaction process by coherent x-ray diffraction imaging. **H. Kim**

Section B

Parc 55 San Francisco

Cyril Magnin III

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

Lignin Conversion & Upgrading

Cosponsored by CARB and ENFL

M. M. Abu-Omar, S. L. Scott, *Organizers*

C. Sievers, *Presiding*

1:00 CATL **151.** Atomic level structure characterization of biomass post Catalytic Depolymerization of Lignin (CDL) by dynamic nuclear polarization-enhanced solid state NMR. **M.M. Abu-Omar**, H. Luo, F. Perras, M. Pruski, N.S. Mosier

1:35 CATL **152.** Reductive conversion of lignin with copper-doped catalysts. **M.B. Foston**, P.C. Ford, D.P. Harper, Y. Gao

2:10 CATL **153.** Divergent pathways for solid-acid catalyzed alkylation of phenol in liquid phase. **H. Shi**, Y. Liu, J. Hu, D.M. Camaioni, J.A. Lercher

2:30 CATL **154.** Aqueous phase transformation of biomass-derived oxygenated compounds over supported tungsten based catalysts. **J.M. Lopez-Nieto**, N. La Salvia, D. Delgado, A. Fernandez-Arroyo, M. Domine

2:50 Intermission.

3:10 CATL **155.** Electrochemical coupling of primary biomass derivatives for the production of second generation platforms for renewable polymer and biofuel applications. L. Wu, **M. Mascal**, T.J. Farmer, S. Pérocheau Arnaud, M. Wong Chang

3:45 CATL **156.** Novel strategies for the catalytic conversion of lignocellulose. **K. Barta**

4:20 CATL **157.** Chemo-enzymatic synthesis of renewable antioxidant additives with tunable polarity from lignocellulose and vegetal oils. **L. Hollande**, J. Beaugrand, P. Ducrot, S. Domenek, F. Allais

4:40 CATL **158.** Electrocatalytic conversion of biologically-produced muconic acid to renewable monomers. J.E. Matthiesen, S. Abdolmohammadi, M. Viswanathan, A. Okerlund, D.R. Raman, **J. Tessonnier**

Section C

Parc 55 San Francisco

Market Street

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Nanocatalysis

Cosponsored by COLL and WCC

C. Kumar, *Organizer*

K. L. Queeney, *Presiding*

1:00 CATL **159.** Recent advances in gold catalysis. **G. Hutchings**

1:30 CATL **160.** Surface chemical transformations and environmental impact of nanoscale complex oxides. **R.J. Hamers**

2:00 Intermission.

2:15 CATL **161.** Chemical patterning of nanoscale topographical features on Si(100). **K.L. Queeney**

2:45 CATL **162.** Modifying catalysts using atomic layer deposition. N. Yang, A.S. Asundi, **S.F. Bent**

3:15 Overview of research accomplishments and acknowledgements. C. Friend

Section D

Parc 55 San Francisco

Cyril Magnin I

Electrocatalysis for Energy Generation & Storage

Fuel Cells, Electrolyzers & Batteries

Cosponsored by ENFL

A. Holewinski, J. Snyder, C. Wang, *Organizers*

H. Xin, *Organizer, Presiding*

A. Holewinski, *Presiding*

1:00 CATL **163.** Synthesis and characterization of thiophene annulated butterfly [2Fe-2S] complexes. **W. Brezinski**, M.O. Talbot, T. Yamamoto, S. Sill, L.M. Stratton, D.L. Lichtenberger, D.H. Evans, R.S. Glass

1:20 CATL **164.** Differential electrochemical x-ray absorption spectroscopy of hydrogen evolution electrocatalysis on metal phosphides. T. Billo, L. Hsu, Y. Lin, **W. Chen**

1:40 CATL **165.** Universal surface engineering of transition metals for hydrogen evolution from water. **Y. Sun**

2:00 CATL **166.** Fundamental understanding of defective carbon-based materials for electrochemical synthesis of hydrogen peroxide. **S. Chen**, Z. Chen, S. Siahrostami, T.R. Kim, D. Nordlund, D. Sokaras, S. Nowak, J.W. To, D.C. Higgins, R. Sinclair, F. Studt, J.K. Norskov, T.F. Jaramillo, Z. Bao

2:20 CATL **167.** Electrocatalytic and thermal catalytic phenol hydrogenation over platinum and rhodium. **N. Singh**, Y. Song, O. Gutiérrez, D.M. Camaioni, C.T. Campbell, J.A. Lercher

2:40 Intermission.

3:00 CATL **168.** Probing the nature of active sites for methanol oxidation with transient isotope kinetics. C. Barnhill, **A. Holewinski**

3:20 CATL **169.** Search for a high efficiently platinum-based mixed-metal anode catalyst for polymer electrolyte membrane fuel cells. **N. Dimakis**, D. Valdez, E.S. Smotkin

3:40 CATL **170.** Ultrasmall intermetallic nanoparticles for enhanced catalytic electro-oxidation. **Z. Qi**, C. Xiao, C. Liu, T. Goh, L. Zhou, R. Maligal Ganesh, Y. Pei, L.A. Curtiss, W. Huang

4:00 CATL **171.** Design of Ni-based electrocatalysts for CO2 electrolysis from first-principles. **X. Gu**, J. Carneiro, E. Nikolla

4:20 CATL **172.** Controlled selectivity towards CO/H2 production during the Co-electrolysis of H2O and CO2 using solid oxide electrolysis cells. **B. Hu**, A. Aphale, W. Song, J.W. Stevenson, S.L. Suib, P. Singh

4:40 CATL **173.** Surface reactions of lithium-oxygen batteries studied under electrochemical control with field ionization methods. H. Valdés Espinosa de los Monteros, K.A. Carpenter, **E. Stuve**

Section E

Parc 55 San Francisco

Cyril Magnin II

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

TECHNICAL PROGRAM

Mechanistic Studies of Catalysis in Photocatalytic & Photoelectrodes

Cosponsored by COLL, ENFL, I&EC and INOR

G. Dukovic, D. Esposito, I. Sharp, *Organizers*

S. Ardo, *Organizer, Presiding*

1:00 CATL **174.** Catalytic reactions on optically excited plasmonic metal nanoparticles. **S. Linic**

1:30 CATL **175.** Plasmon-Driven photoelectrochemical cells for artificial photosynthesis. **J. DuChene**, G. Tagliabue, A.J. Welch, Q. Yang, K. Reidy, A.R. Davoyan, C. Hsiow, H. Atwater

1:45 CATL **176.** Hot electron and surface plasmon-driven water splitting on Au nanoparticles/TiO2 nanotube arrays. **S. Moon**, K. Goddeti, E. Gwag, J. Park

2:00 CATL **177.** Investigation of plasmon-enhanced photocatalytic CO2 reduction using nanostructured heterogeneous Ag and Cu catalysts. **Y. Kim**, E. Creel, E. Corson, F. Qiu, J. Urban, B.D. McCloskey, R. Kostecki

2:15 CATL **178.** Effect of the application of a non-resonant electric field on the photodissociation dynamics of HBr. **M. Sneha**, Y.H. Lai, J. Meiser, K.I. Hilsabeck, R.N. Zare

2:30 CATL **179.** Photoelectrochemical hydrogen evolution reaction with quantum yield exceeding 100% via MEG. **Y. Yan**

2:45 Intermission.

3:00 CATL **180.** Fate of carbon dioxide in water-rich fluids under extreme conditions. **G.A. Galli**, D. Pan

3:30 CATL **181.** Three distinct nature of surface-bound atomic hydrogen and their role in dictating product selectivity in artificial photosynthesis reactions. **S. Poudyal**, S. Laursen

3:45 CATL **182.** Charge transfer processes in catalyzed semiconductor photoelectrodes. **S.W. Boettcher**

4:15 CATL **183.** Intrinsic carrier transport and photocatalytic behavior in single crystallie bismuth vanadate thin film solar water splitting photoanodes. W. Zhang, D. Yan, **M. Liu**

4:30 CATL **184.** Exceptionally stable molybdenum disulfide protection schemes for silicon photocathodes. **L. King**, T. Hellstern, T.F. Jaramillo

Section F

Parc 55 San Francisco

Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

1:00 CATL **185.** Augmenting reaction mechanisms for improved computational catalyst screening. **L. Grabow**

1:20 CATL **186.** Standard states of adsorbates on surfaces. **A. Savara**, C.T. Campbell

2:00 CATL **187.** Understanding the role of anionic dopants on Pd for hydrogen production from formic acid. **P. Sautet**, P. Wang, S. Steinmann, C. Michel, G. Fu

2:40 CATL **188.** Stabilization of catalytically active Cu+ surface sites on titanium–copper mixed-oxides. **D.J. Stacchiola**

3:00 CATL **189.** Mechanistic requirements of hydrogen addition to carbonyl compounds. F. Lin, J. Shangguan, Z. Wu, **Y. Chin**

3:40 CATL **190.** Mechanistic origins of unselective oxidation products in the conversion of propylene to acrolein. **L. Bui**, A. Bhan

4:20 CATL **191.** Calculating free energy of atomic oxygen adsorbed on late transition metal surfaces. **K. Frey**

4:40 CATL **192.** First-principles study of water-gas shift reaction on cobalt: Microkinetic modeling of a system with strong coverage effects. **W. Luo**, A.R. Asthagiri

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Synthesis & Characterization of Materials for Energy Applications

In Operando & Surface Sensitive Analysis

Sponsored by ANYL, Cosponsored by CATL

C1 Catalysis

Sponsored by ENFL, Cosponsored by CATL

Catalytic Materials from Molecular Insight

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Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Catalysts for Selective Chemical Transformations

Sponsored by COLL, Cosponsored by CATL

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

Sustainability in Electrocatalytic Fuel & Chemical Production

Sponsored by INOR, Cosponsored by CATL

TUESDAY MORNING

Section A

Parc 55 San Francisco

Cyril Magnin III

Advanced X-Ray Techniques for Catalyst Characterization

New Methodologies

Cosponsored by PHYS

A. M. Karim, *Organizer*

S. R. Bare, *Organizer, Presiding*

8:00 CATL **193.** Ex-situ profiling of TiO2 thin film growth: An XRD study using synchrotron radiation. **K.A. Kulinski**, D. Steckhahn, B. Gunn, C. Tassone, A.S. Ichimura

8:20 CATL **194.** Characterization of catalysts with operando x-ray spectroscopy. **D. Sokaras**

9:00 CATL **195.** *Operando* electrochemical grazing incidence x-ray absorption and diffraction for the CO2 reduction reaction. **J. Feaster**, M. Farmand, J. Lin, A. Landers, S. Fackler, R. Davis, A. Mehta, J. Yano, T.F. Jaramillo, W. Drisdell

9:20 CATL **196.** Advanced X-ray spectroscopic tools for operando catalysis studies at the National Synchrotron Light Source-I. **E. Stavitski**

9:50 CATL **197.** Using organometallic model complexes to assist in interpreting x-ray absorption spectra of single-site catalysts. A.(. Getsoian, J. Camacho-Bunquin, G. Zhang, **A. Hock**

10:20 CATL **198.** Analytical XAFS and XES on the benchtop in research groups, industrial testing facilities, and teaching labs. **G. Seidler**, E. Jahrman, W. Holden, A. Ditter, O. Hoidn, L. Bradshaw, S.A. Kozimor, J. Sieber, D. Mortensen

10:50 Discussion.

Section B

Parc 55 San Francisco

Powell I/II

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

Carbohydrate Processing & Upgrading of Biomass-Derived Molecules

Cosponsored by CARB and ENFL

M. M. Abu-Omar, S. L. Scott, *Organizers*

J. Tessonnier, *Presiding*

8:00 CATL **199.** Intensified oxidative processes for biomass conversion to chemicals. **B. Subramaniam**, M. Lundin, A.M. Danby, X. Zuo

8:35 CATL **200.** New fine chemical building blocks from lignin via stabilization of reactive intermediates from the C-2 acidolysis pathway. **J.G. De Vries**, K. Barta, P.J. Deuss

9:10 CATL **201.** Deactivation paths during hydrodeoxygenation of aromatic oxygenates over Pt/H-BEA. C. Okolie, G. Foo, M.V. Rodrigues, M. Yung, **C. Sievers**

9:45 Intermission.

10:05 CATL **202.** Recent advances in biomass conversion for bioproducts and fuels. **D.G. Vlachos**, B. Saha, P.J. Dauenhauer, W. Fan, M. Tsapatsis, S. Caratzoulas

10:40 CATL **203.** Ru-based heterogeneous catalysts for levulinic acid hydrogenation: On the influence of catalyst composition, synthesis and feed impurities. P. Bruijnincx, **B.M. Weckhuysen**

11:15 CATL **204.** Observing biomass conversion at solid-liquid interfaces using operando solid-state NMR spectroscopy. **L. Qi**, A. Chamas, D.W. Hoyt, E. Walter, N. Washton, M. Foston, S.L. Scott

11:35 CATL **205.** Muconic acid isomerization strategies: The role of water (friend or foe?). **J. Carraher**, J. Tessonnier

Section C

Parc 55 San Francisco

Market Street

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Single Crystal Catalysis

Cosponsored by COMP

T. Bligaard, C. M. Friend, C. Kumar, *Organizers*

J. Rodriguez, *Presiding*

8:00 Introductory Remarks.

8:15 CATL **206.** Heterogeneous photochemical processes on metal oxides. A.S. Crampton, F. Xu, E. Kaxiras, L. Cai, X. Zheng, **C.M. Friend**

8:45 CATL **207.** On the active site model in computational catalyst screening. **K.U. Reuter**

9:15 Intermission.

9:30 CATL **208.** Modifications of Pt single crystal surfaces for designing ideal electrochemical interfaces in PEFCs. **K. Kodama**, R. Jinnouchi, A. Shinohara, Y. Morimoto

10:00 CATL **209.** Mechanistic studies of the HDO of lignin-derived oxygenates on PtZn: From single crystals to high surface area catalysts. **J.M. Vohs**, D. Shi

10:30 Intermission.

10:45 CATL **210.** Decoding the rich behaviour of single atom alloys and identifying opportunities for catalyst design. **M. Stamatakis**

11:15 CATL **211.** Inverse oxide/metal systems and fundamental studies in heterogeneous catalysis. **J. Rodriguez**, P. Liu, J. Graciani, S.D. Senanayake, D.J. Stacchiola, J.F. Sanz

Section D

Parc 55 San Francisco

Cyril Magnin I

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Molecular & Bio-Inspired Photocatalysts

Cosponsored by COLL, ENFL, I&EC and INOR

S. Ardo, D. Esposito, I. Sharp, *Organizers*

G. Dukovic, *Organizer, Presiding*

8:00 CATL **212.** Photocatalytic reduction of CO2. **C.P. Kubiak**, P. Cheung, A. Zhanaidarova

8:30 CATL **213.** Catalytic light-driven reductive transformations mediated by cobalt complexes. **J. Lloret Fillol**, A. Call, C. Casadevall, F. Acuña-Pares, A. Casitas Montero, M. Claros

8:45 CATL **214.** Photoinduced proton-coupled electron transfer in solvated molecular systems and photoreceptor proteins. **S. Hammes-Schiffer**

9:15 CATL **215.** π-Hole–π interaction promoted photocatalytic hydrodefluorination via inner-sphere electron transfer. **J. Lu**, N. Khetrapal, J. Johnson, X.C. Zeng, J. Zhang

9:30 Intermission.

‡ *Cooperative Cosponsorship*

9:45 CATL **216.** Study of light-driven catalysis by enzyme-nanoparticle hybrids. **P.W. King**, K.A. Brown, D. Harris, M. Wilker, H. Hamby, S. Keable, N. Khadka, L.C. Seefeldt, J. Peters, G. Dukovic

10:15 CATL **217.** Photocatalytic NADH-analog systems for fuel-forming reactions. **K. Glusac**

10:30 CATL **218.** Molecular surface coatings for semiconductor photoelectrochemistry and photocatalysis. **G.F. Moore**, A.M. Beiler, D. Khusnutdinova, B.L. Wadsworth

11:00 CATL **219.** Atomic layer-deposited cobalt oxide stabilizes dye-sensitized photoanodes for improved photoelectrochemical water splitting. **P. Xu**, Y. Hu, C. Gray, I. Sharp, T.E. Mallouk

11:15 CATL **220.** Design of visible light organic photoredox catalysts for the synthesis of polymers and small molecules. **C. Lim**, R.M. Pearson, J.C. Theriot, B.G. McCarthy, M.D. Ryan, H. Yang, C. Musgrave, G. Miyake

11:30 CATL **221.** Design of photoredox catalysts for efficient organocatalyzed atom transfer radical polymerization. **C. Musgrave**, C. Lim, J.C. Theriot, G. Miyake, M.D. Ryan, B.G. McCarthy, S. Sartor, N.H. Damrauer

Section E

Parc 55 San Francisco

Cyril Magnin II

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Cosponsored by ENVR and I&EC

M. A. Banares, M. Guerrero-Perez, F. Tao, *Organizers*

G. Rupprechter, *Presiding*

8:00 CATL **222.** Molecular catalysis science. Nanoparticle synthesis, and instrument development for characterization under reaction conditions. Conquering catalytic complexity. **G.A. Somorjai**

8:40 CATL **223.** Operando studies of working catalysts by synchrotron-based XPS and XAS at atmospheric pressure. **G. Rupprechter**, K. Foettinger, C. Rameshan

9:20 Intermission.

9:40 CATL **224.** Operando spectroscopy from the perspective of SUNCAT and SSRL. **S.R. Bare**

10:20 CATL **225.** Bridging the material and pressure gaps in synchrotron based photoelectron in-situ/operando studies. **L. Gregoratti**, M. Amati, H. Sezen

Section F

Parc 55 San Francisco

Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

Electrons

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

8:00 CATL **226.** Surface thermodynamics and kinetics of perovskite oxides. L. Zhang, D. Müller, Z. Guan, C. Gopal, M. Monti, W. Chueh, **A. Vojvodic**

8:20 CATL **227.** NO electrochemical reduction on transition metal electrocatalysts: A DFT approach. H. Chun, K. Honkala, V. Apaja, A.Z. Clayborne, **J. Greeley**

9:00 CATL **228.** Direct synthesis of H2O2: Competing reaction pathways depend differently on surface structure. N. Wilson, P. Priyadarshini, **D. Flaherty**

9:40 CATL **229.** When modelling bridges electrocatalysis and heterogeneous catalysis: The case of the formic acid decomposition. **S.N. Steinmann**, C. Michel, P. Sautet

10:00 Intermission.

10:20 CATL **230.** Enhancing rates of redox reactions with surface-induced solvent effects. **R.C. Remsing**

10:40 CATL **231.** Reaction mechanisms for the electrochemical reduction of CO2 on the Cu(100) surface from quantum mechanics free energy calculations with explicit water. **T. Cheng**, H. Xiao, W.A. Goddard

11:00 CATL **232.** Silicon surface termination affects electrolyte reduction pathways as probed by in situ sum frequency generation vibrational spectroscopy. **Y. Horowitz**, H. Han, G.A. Somorjai

11:20 CATL **233.** Computational investigation of secondary electron emission and other mechanisms involved in plasma-assisted dry methane reforming using nickel catalysts. **A. Sirjoosingh**, G.C. Schatz

Synthesis & Characterization of Materials for Energy Applications

Fundamental & Molecular Models for Advanced Energy Materials

Sponsored by ANYL, Cosponsored by CATL

Functional Porous Materials for Sustainable Energy

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Advanced Materials & Technologies for Solar Energy Conversion & Storage

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Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Surface Science of Functional Interfaces

Sponsored by COLL, Cosponsored by CATL

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

TUESDAY AFTERNOON

Section A

Parc 55 San Francisco

Cyril Magnin III

General Papers

S. L. Scott, *Organizer*

E. Nikolla, *Organizer, Presiding*

1:00 CATL **234.** Advancing energy applications with nanoscale hybrid catalysts: The key concept of exploiting interfaces. **P. Fornasiero**, M. Prato, F. Paolucci, M. Bonchio, R.J. Gorte

1:20 CATL **235.** Efficient biomass transformation to chemicals and biofuel catalyzed by ordered mesoporous solid acid. **C. Carrie**, J. Boravilas, A. Masoumi, B. Kanjilal, F. Liu, C. Slater, M.J. Savelski, J.F. Stanzione, I. Noshadi

1:40 CATL **236.** Structure-Activity relationships in m-cresol hydrodeoxygenation over platinum catalysts. **J.A. Hunns**, K. Wilson, A.F. Lee, M. Watson

2:00 CATL **237.** Enhanced production of aromatics from biomass upgrading over in-framework Ga-ZSM5 catalysts via A systematic study. **M. Xu**, C. Mukarakate, B.G. Trewyn, R.M. Richards

2:20 CATL **238.** Investigating lignin disassembly pathways through modifications of Cu-doped porous metal oxide catalysts. **M.A. Chui**, G. Metzker, C.M. Bernt, A. Tran, P.C. Ford

2:40 CATL **239.** Selective non-oxidative ethanol dehydrogenation on dilute NiCu alloys. **N. Janvelyan**, J. Shan, H. Li, J. Liu, T. Egle, J. Ye, M.M. Biener, J. Biener, M. Flytzani-Stephanopoulos, C.M. Friend

3:00 Intermission.

3:15 CATL **240.** Pt-catalysed hydrodeoxygenation of lignin monomers: Understanding of factors affecting the catalyst performance. **A. Shivhare**, A.F. Lee, K. Wilson, J.A. Hunns, C.M. Parlett, M. Isaacs

3:35 CATL **241.** Effect of post-treatment on structure and catalytic activity of CuCo-based materials for glycerol oxidation. **G. Dodekatos**, H. Tuysuz

3:55 CATL **242.** *Ex-situ* catalytic fast pyrolysis of lignocellulosic biomass over Pt/TiO2: Fundamental insight to large bench scale validation. **M. Griffin**, G.A. Ferguson, C. Mukarakate, M.J. Biddy, D.A. Ruddy, R.J. French, F.G. Baddour, G. Beckham, J. Schaidle

4:15 CATL **243.** Transition metal phosphide catalysts for methanol synthesis from CO and CO2. **M.S. Duyar**, J. Snider, E. Valle, T.F. Jaramillo

4:35 CATL **244.** Thermodynamic and kinetics studies on site requirements for aldol addition over differently prepared TiO2 catalysts. **H. Zhang**, D. Flaherty

Section B

Parc 55 San Francisco

Powell I/II

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

Cosponsored by CARB and ENFL

S. L. Scott, *Organizer*

M. M. Abu-Omar, *Organizer, Presiding*

1:00 CATL **245.** Acrylonitrile production from biomass-derived intermediates. **G. Beckham**, M.J. Biddy, D. Brandner, A. Bratis, J.R. Dorgan, T. Eaton, E. Karp, L. Manker, W. Michener, D. Salvachua, V. Sànchez i Nogué, E. Tan, D. Vardon, X. Wang

1:35 CATL **246.** Catalytic reductions of oxygenates with oxophilic metal complexes as catalysts. **A.D. Sadow**

2:10 CATL **247.** Selective hydrogenation of xylose to xylitol in the presence of Co/SiO2 catalysts. **K. De Oliveira Vigier**, M. Audemar, F. Jérôme, S. Royer

2:30 CATL **248.** Vanadium-catalyzed aerobic oxidative C-C bond cleavage of 1,2-diols: A coupled theoretical and experimental study of an unprecedented direct two-electron oxidation. C. Diaz-Urrutia, **P. Fleurat-Lessard**, C. Michel, S. Gorelsky, I. Korobkov, A. Martinez, R. Baker

2:50 Intermission.

3:10 CATL **249.** C6 diacids from homocitric acid lactone using relay heterogeneous catalysis. I. Thapa, S. Ntais, E. Baranova, M.K. Lau, C. Hass, J. Millis, **R. Baker**

3:45 CATL **250.** Catalytic approaches to complex molecules from carbohydrate biomass. **M.R. Gagne**

4:20 CATL **251.** Evolution of a heterogeneous Cu-based lignin hydrogenolysis catalyst in supercritical methanol. **Z. Jones**, J.A. Barrett, J. Zhang, P.C. Ford, S.L. Scott

4:40 CATL **252.** Anatase TiO2 activated by gold particles for selective hydrodeoxygenation of guaiacol to phenolics. **Z. Zhang**, J. Mao, J. Zhou, Z. Xia, Z. Wang, Z. Xu, W. Xu, P. Yan, K. Liu, X. Guo

Section C

Parc 55 San Francisco

Market Street

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Electrocatalysis

Cosponsored by COMP

T. Bligaard, C. M. Friend, C. Kumar, *Organizers*

A. Vojvodic, *Presiding*

1:00 CATL **253.** Analysis of the mechanism of electrochemical oxygen reduction and development of Ag- and Pt-alloy catalysts for low temperature fuel cells. **S. Linic**

1:30 CATL **254.** Engineering complex, layered metal oxides for high temperature electrochemical oxygen reduction and evolution. **E. Nikolla**

2:00 Intermission.

2:15 CATL **255.** Transition-metal compounds as electrocatalysts. **A. Vojvodic**

2:45 CATL **256.** Improving our understanding of electrochemical reaction barriers. **A. Peterson**, P. Lindgren, G. Kastlunger, M. El Khatib

3:15 Intermission.

3:30 CATL **257.** Spectroscopy and microscopy at the solid-vapor and solid-liquid interface. **M. Salmeron**

4:00 CATL **258.** Machine learning approach to electrocatalyst discovery. **H. Xin**

Section D

Parc 55 San Francisco

Cyril Magnin I

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Novel Photocatalytic & Photoelectrode Materials

Cosponsored by COLL, ENFL, I&EC and INOR

S. Ardo, G. Dukovic, D. Esposito, *Organizers*

I. Sharp, *Organizer, Presiding*

1:00 CATL **259.** Photocatalysis induced by direct electron emission from diamond surfaces. **R.J. Hamers**

1:30 CATL **260.** High throughput discovery of solar fuels photoanodes. **J. Gregoire**

2:00 CATL **261.** Solar fuels photoanodes prepared by inkjet printing of copper vanadates. **P. Newhouse**, D. Boyd, A. Shinde, D. Guevarra, L. Zhou, E. Soedarmadji, G. Li, J. Neaton, J. Gregoire

2:15 CATL **262.** Polymer photocatalysts for water splitting; lessons from experiment and theory. **M.A. Zwijnenburg**, R. Sprick, D. Adams, A.I. Cooper

2:30 CATL **263.** Molybdenum disulfide as a protection layer and catalyst for gallium indium phosphide solar water splitting photocathodes. **R.J. Britto**, J. Young, D. LaFehr, J. Benck, C. Hahn, T.G. Deutsch, T.F. Jaramillo

2:45 Intermission.

3:00 CATL **264.** Is it photocatalysis or is it photosynthesis? Developing design criteria for enhanced solar energy conversion and photocatalytic devices. **F.E. Osterloh**, Z. Zhao, M.A. De Melo Junior

3:30 CATL **265.** Sculpting photocatalysts on the nano scale. **L. Amirav**

4:00 CATL **266.** Multicatalytic, light-driven upgrading of butanol to 2-ethylhexenal and hydrogen under mild aqueous conditions. **G. Hafenstine**, K. Ma, A.R. Harris, O. Yehezkeli, E. Park, D. Domaille, J. Cha, A.P. Goodwin

4:15 CATL **267.** Nanocrystalline CoO photocatalyst: Role of facets in overall water splitting. **K. Park**, A. Kolpak

4:30 CATL **268.** Nanostructured non-precious metal silicon photocathodes for solar water splitting. **T. Hellstern**, P. Chakthranont, L. King, I. Narkeviciute, R.J. Britto, D. Palm, C. Hahn, T.F. Jaramillo

Section E

Parc 55 San Francisco

Cyril Magnin II

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Cosponsored by ENVR and I&EC

M. Guerrero-Perez, F. Tao, *Organizers*

M. A. Banares, *Organizer, Presiding*

1:00 CATL **269.** Operando beyond catalysis: Spectroscopic characterization of separation measurements in membranes combined with modelling. **M. Daturi**, C. Le Guillouzer, P. Bazin, S. Thomas, A. Vimont, G. Clet

1:40 CATL **270.** Operando membrane spectroscopy: A novel technique for identifying membrane structure-function relationships. **C. O'Brien**, I. Lee, Z. Dunbar

2:00 CATL **271.** Modeling catalysts under a pressure of gas. **P. Sautet**

2:40 Intermission.

3:00 CATL **272.** New aspects of environmental TEM in catalyst chemistry. **S. Takeda**, R. Aso, N. Kamiuchi, H. Yoshida, K. Soma

3:40 CATL **273.** Development of a reaction cell for in-situ/operando studies of surface of a catalyst under a reaction condition and during catalysis. **F. Tao**

Section F

Parc 55 San Francisco

Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

Organic Oxygenates

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

1:00 CATL **274.** Elucidation of the mechanism and kinetics of catalyzed reactions: Application of experimental and theoretical approaches. **A.T. Bell**

1:40 CATL **275.** Mechanisms of lignin and furan derivative upgrade on metal surfaces. **D.G. Vlachos**, G. Gu, G. Jenness

2:20 CATL **276.** Catalysis in a cage: The dynamic nature of active copper sites in zeolites during NOx SCR with ammonia. A.A. Parekh, C. Paolucci, I. Khurana, J.D. Albarracin-Caballero, J.R. Di Iorio, A. Shih, H. Li, S. Li, A. Yezerets, W.N. Delgass, J.T. Miller, F. Ribeiro, W.F. Schneider, **R. Gounder**

3:00 CATL **277.** Theoretical investigation of the catalytic hydrodeoxygenation of levulinic acid over Ru(0001) surface. **A. Heyden**

3:40 CATL **278.** Collision theory in liquids and the molecular origin of the selectivity difference between AuPd and Pd for benzylic alcohol oxidation. **A. Savara**, C.E. Chan-Thaw, I. Rossetti, L. Prati, A. Villa

4:00 CATL **279.** Hydrodeoxygenation of phenol through FeXMo2-XP bimetallic phosphide catalyst: A Density Functional Theory (DFT) study. **V. Jain**, N. Rai

4:20 CATL **280.** Characterization of active centers in the zeolite SSZ-13. **F. Goeltl**, I. Hermans, M. Mavrikakis

Synthesis & Characterization of Materials for Energy Applications

Novel Architectures, Materials & Synthetic Routes/In Operando & Surface Sensitive Analysis

Sponsored by ANYL, Cosponsored by CATL

ACS Award Lectures

Sponsored by COLL, Cosponsored by CATL and WCC

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

TUESDAY EVENING

Section A

Moscone Center

Hall D

Poster Session

E. Nikolla, S. L. Scott, *Organizers*

6:00 - 8:00

CATL **281.** Acetone sensing mechanism of PdO at temperatures below 250oC. **C. Tsai**, Y. Chen, I. Cheng, F. Pan

CATL **282.** Design of highly-stable and reactive Pt catalysts dispersed on CeO2-TiO2 interface. **M. Yoo**, H. Ha, H. Kim

CATL **283.** DFT Study on single atom Au/Co3O4(111) catalyzing CO oxidation. **W. Hu**, **X. Cao**, P. Hu

CATL **284.** DFT corroborated study for the synthesis of cyclic carbonate from epoxide and CO2 using a mixed Cu(II) amino acid-imidazolate MOF catalyst. **D. Park**, A.C. Kathalikkattil, H. Woo

CATL **285.** Degradation of herbicide Basagran 480 with iron oxide nanoparticles. **M. Ocampo**, L. Payan, I. Hernández, V. Garibay, R. Suárez, L. González

CATL **286.** Structure and catalytic activity of molybdenum carbide and oxycarbide nanoparticles in ZSM-5 for natural gas conversion to aromatics. **Y. Zheng**

CATL **287.** Enhanced activity and stability of CuO-ZnO-ZrO2 catalyst by addition of graphene oxide for CO2 hydrogenation to methanol. **T. Witoon**, S. Bumrungsalee, W. Donphai, M. Chareonpanich, J. Limtrakul

CATL **288.** CO Adsorption induced Pd-Au swapping in Pd-core@Au-shell nanoparticles. **H. An**, H. Ha, M. Yoo, H. Kim

CATL **289.** Magnesium modified HZSM-5 with superior on-stream stablility for fluid catalytic cracking naphtha hydro-upgrading. Q. Lü, **Y. Yue**, Y. Zhou, H. Liu, **X. Bao**

CATL **290.** Higher alcohol synthesis via Fischer-Tropsch metal surface modification of MoP catalyst. **E. Valle**, M. Duyar, T.F. Jaramillo

CATL **291.** Efficient reversible hydrogen carrier system based on amine reforming of methanol. **S. Kar**, **J. Kothandaraman**, R. Sen, A. Goeppert, G. Olah, S.G. Prakash

CATL **292.** Insights from a QM/MM Investigation of ethane dehydrogenation pathways on Ga/H-MFI. **E. Mansoor**, M.P. Head-Gordon, A.T. Bell

CATL **293.** Nanostructured carbon decorated molybdenum sulfide for the catalytic decomposition of water to produce hydrogen and for supercapacitive applications. **J. Candler**, K.S. Siam, P.K. Kahol, R. Gupta

CATL **294.** Methane pyrolysis using catalytic melts for CO2 free hydrogen production. **D.C. Upham**, M.J. Gordon, H. Metiu, E.W. McFarland

CATL **295.** Cobalt-nitrogen doped 3D porous carbon prepared with self-generated nanoparticles as sacrificial templates for hydrogen generation. **Z. Zhang**, F. Wang, S. Yang, M. Dou, J. Ji

CATL **296.** Heterogeneous organo-catalysis: Sustainable pathway to furanics from biomass. **S. Verma**, R.S. Varma

CATL **297.** Methanol synthesis from CO2 and H2 on Au/ZnO: Mechanistic insights from the analysis of adsorbed species formed under reaction conditions. **A.M. Abdel-Mageed**, D. Widmann, A. Rezvani, R.J. Behm

CATL **298.** Competition between Reverse Water Gas Shift (RWGS) reaction and CO2 methanation on Ru/TiO2: Temperature induced structural changes. **A.M. Abdel-Mageed**, D. Widmann, K. Wiese, A. Hauble, R.J. Behm

CATL **299.** Studies on preparation and catalytic cracking performance of small particle USY zeolite. **G. Wang**, S. Cui, B. Liu

CATL **300.** Environmental TEM study of nanoparticles using modified *in-situ* E-TEM chips. **Q. Wu**, **J. Cen**, C.J. Ridge, D. Zakharov, X. Tong, M. Lindsay, A. Orlov

CATL **301.** Lower valence metal doping of bulk Cr2O3: Charge compensation and oxygen vacancy formation. J.J. Carey, **M. Nolan**

CATL **302.** Hierarchical muticomponent catalysts: Structure design, function realization and catalytic applications. **G. Wang**, H. Gao, S. Fan, D. Jia, J. Wang, L. Tan, W. Dong

CATL **303.** Catalytic conversion of sugar stream to hydrocarbons. **A.B. Padmaperuma**, M.A. Lilga, D.L. Auberry

CATL **304.** Withdrawn.

CATL **305.** Carbon dioxide capture and conversion using CNT based catalysts. Z. Zhou, **K.J. Stowers**

CATL **306.** Flower-like CuO/titania nanotube arrays for water splitting application. **W. Chiu**, H. Chiu, C. Lee

CATL **307.** Porous structure-dependent electrocatalytic activity of cobalt and nitrogen co-doped carbon electrocatalyst for oxygen reduction reaction. **Y. Song**, M. Dou, X. Wen, F. Wang

‡ *Cooperative Cosponsorship*

CATL **308.** Withdrawn.

CATL **309.** Cu/ZnO core-shell catalysts for methanol synthesis from CO2: Structure-Activity relationship. **R. Gaikwad**, D. Koziej, M. Niederberger, A. Urakawa

CATL **310.** Preparation of carbon molecular sieve composite membrane for N2/F-gases separation. **S. Kim**, P. Lee, S. Nam, H. Park, Y. Park

CATL **311.** 2D-Nanosheets with palladium nanoparticles for C-C coupling reactions. **D. Yim**, F. Raza, J. Park, H. Kim, H. Lee, J. Kim

CATL **312.** Benzene in olefin metathesis by Ru-based catalysts. **A. Poater**, J. Poater, R. Chauvin

CATL **313.** One-step conversion from Ni/Fe polyphthalocyanine to N-doped carbon supported Ni-Fe nanoparticles for highly efficient water splitting. **F. Wang**, Z. Zhang, Y. Qin, M. Dou, J. Ji

CATL **314.** Direct conversion of olefins and CO2 over a supported catalyst. C. Nguyen-Sorenson, **K.J. Stowers**

CATL **315.** Synthesis of hierarchical zeolite Y by acid dealumination for cracking reactions. **K. Sunny**, A. Dabbawala, I. Ismail, M. Khaleel, **S. Al Hassan**

CATL **316.** Control synthesis of nano-sized Zeolite-Y using starch gel as the sole template for catalytic cracking applications. **K. Youssed**, A. Dabbawala, I. Ismail, M. Khaleel, **S. Al Hassan**

CATL **317.** Withdrawn.

CATL **318.** Metal modified zirconium hydrogen phosphate for the oxygen evolution reaction. **J. Sanchez**, M. Ramos, I. Narkeviciute, J.L. Colon, T.F. Jaramillo

CATL **319.** Control of catalyst deactivation by wet methods. **G. Owusu**, A. Baker, A. Alba-Rubio

CATL **320.** Synthesis of aggregated organosilica nanotubes and their application in catalysis. **A. Manchanda**, C. Gunathilake, M.E. Gangoda, P. Ghimire, M. Jaroniec, M. Kruk

CATL **321.** Probing oxidation states of metal/SiO2 hybrid nanocatalyst under CO oxidation with in situ FTIR spectroscopy. **S. Oh**, S. Back, W. Doh, S. Moon, J. Kim, Y. Jung, J. Park

CATL **322.** Atomic structure of the Pt/γ-Al2O3 interface through a combined experiment and theory approach: A model catalyst study. **H. Ayoola**, C.S. Bonifacio, Q. Zhu, J. Kas, K. Kisslinger, D. Su, E. Stach, J.J. Rehr, W. Al-Saidi, J. Yang

CATL **323.** Density functional theory study of reactivity of CeO2-supported Pt nanoparticles for the CO oxidation. **H. Ha**, M. Yoo, H. An, H. Kim

CATL **324.** Withdrawn.

CATL **325.** Withdrawn.

CATL **326.** Sacrificial coating strategy toward enhancement of metal-support interaction for ultrastable Au nanocatalysts. **W. Zhan**, Y. Guo, Y. Guo, W. Li

CATL **327.** One-pot growth of 3D reduced graphene oxide foams embedded with MoS2 and Ni-doped MoS2 nanocatalysts for hydrogen evolution reaction. **C. Li**, J.B. Grantham, W. Zhao

CATL **328.** Reactions of enolized carboxylic acids with electrophiles on metal oxide surface. **A. Cohen**, A. Ignatchenko, O.A. Fraser

CATL **329.** Selective hydrogenation of dienes and trienes using partially poisoned palladium nanoparticle catalysts. **T. Chen**, Y. Shon

CATL **330.** Screening of binary alloy thin films for electrochemical CO2/CO reduction. **S. Nitopi**, L. Wang, D.C. Higgins, C. Morales Guio, A. Landers, T. Hatsukade, C. Hahn, T.F. Jaramillo

CATL **331.** Multifunctional homogeneous-heterogeneous polymer catalysts for biomass conversion. **S. Kalidindi**, A. Alba-Rubio

CATL **332.** Graphene-based porous adsorbents for CO2 capture. **H. Abbo**, G. Kelly, S. Titinchi

CATL **333.** Vapor phase deposition of silver-copper nanoparticles for the oxygen reduction reaction. **B. Gibbons**, D.C. Higgins, M. Wette, B. Clemens, T.F. Jaramillo

CATL **334.** Facile *in-situ* synthesis of amorphous manganese oxides nanosheets on polyester fibers and their application in oxidative decomposition of formaldehyde. **L. Jinge**, P. Zhang

CATL **335.** Tungsten doped manganese oxides as efficient catalysts for removing formaldehyde at ambient temperature. **F. Liu**

CATL **336.** Reaction study of MnOX nanoparticles on Co3O4: New route to low pressure CO2 conversion. **S. Dalieh**, W. Ralston, W. Liu, G. Melaet, G.A. Somorjai

CATL **337.** Effect of acid sites on platinum catalyzed C-C bond transformations. **A. Flores-Betancourt**, G.A. Somorjai, J. Thierry

CATL **338.** Aqueous-phase Pt(111)-catalyzed methanol dehydrogenation thermodynamics and kinetics using a combined DFT/MD model. **C. Bodenschatz**, R. Getman

CATL **339.** Surface modification scanning by pretreatment on FePt alloy nanoparticles for CO oxidation. **X. Liu**, H. Zhu, S. Dai, M. Chi, G. Lu

CATL **340.** Enhanced catalytic performance of Pt/TiO2 catalyst in water gas shift reaction by incorporation of PRGO. **J. Park**, R. Hwang, K. Yi

CATL **341.** Kinetics of Ni-based oxygen carrier with MgO contents for chemical looping combustion. **J. Park**, R. Hwang, K. Yi

CATL **342.** Alginate as Ag3PO4/g-C3N4 immobilizing agents applied in the photodegradation of diclofenac under visible irradiation. **Z. Wei**, J. Shi, H. Deng

CATL **343.** Structure of directing agent and its effect on fabrication of nano-crystalline Y aggregates. **X. Zhao**, H. Zhang, R. Liu, X. Meng, Y. Gong, Z. Li

CATL **344.** Selective catalytic oxidation of ammonia over MnOx-TiO2 mixed oxides. **W. Li**, Y. Guo, Y. Guo, W. Zhan

CATL **345.** Single polymer chain supported well-defined and multifunctional catalyst design for high precession olefin polymerization. **A. Thakur**, M. Terano, T. Taniike

CATL **346.** Use of iron ore as Fischer Tropsch synthesis catalyst. K. Ramutsidela, L. Xiaojun, **X. Liu**, D. Hildebrandt

CATL **347.** Withdrawn.

CATL **348.** On the mechanism of the catalytic oxidation of 1,2-dichloroethane over CeO2: A DFT+U study. **L. Yin**

CATL **349.** Preparation of todorokite-type manganese dioxide and its application in gaseous ozone removal. **Y. Liu**, P. Zhang

CATL **350.** Supporting the development of palladium catalysts in the direct heteroarylation synthesis of organic pi-conjugated materials. **S.M. McAfee**, A. Hendsbee, A. Payne, G. Welch

CATL **351.** Kinetic study and multi-objective optimization of Fischer-Tropsch synthesis performance over Co-based catalyst using evolutionary optimization algorithm. **N. Moazami**, M. Wyszynski, K. Rahbar, A. Tsolakis

CATL **352.** Phosphrous modification of ZSM-5 extrudates for prolonging catalytic lifetime in Methanol to Propene (MTP) reaction. **Y. Song**, J. Li, Y. Shang, Z. Zhao, X. Zhao, T. Ma, L. Zhang, Y. Gong

CATL **353.** Influence of Al zoning in ZSM-5 on catalytic cracking of hexane. **T. Ma**, Z. Geng, Y. Song, L. Zhang, Y. Shang, Y. Gong

CATL **354.** Synthesis of three-dimensionally ordered macroporous La1-xCexNiO3-δ and their excellent catalytic performance for the ethanol steam reforming. **J. Shao**, Y. Li

CATL **355.** Doped Tansission metal oxide nano-catalysts used to improve performance of hybrid-model vehicle. P. Villarreal, S. Bashir, **J.L. Liu**

CATL **356.** One-pot synthesis with size-control of palladium nanoparticles on reduced graphene oxide by spontaneous redox deposition. **X. Zhang**, W. Ooki, Y.R. Kosaka, A. Okonogi, T. Kondo, J. Nakamura

CATL **357.** Synthesis of wrinkled mesoporous titanosilicate for selective oxidation of cyclohexene. Z. Wang, **K.J. Balkus**

CATL **358.** Enhancing oxidation acitivity ceria through VOx-, CrOx- and MnOx-modification of CeO2 (111). **M. Nolan**, V. Ganduglia-Pirovano

CATL **359.** Microwave-assisted selective hydrogenation of furfural to furfuryl alcohol employing a green and noble metal-free Cu catalyst. **J. Lopez-Sanchez**, P.N. Romano, J.M. de Almeida, Y. Carvalho, P. Priecel, E. Falabella S. Aguiar

CATL **360.** Experimental verification of the poisoning effect of SO2 on the CO2 permeation through a Ce0.8Sm0.2O1.9-carbonate dual phase membrane. **T. Chen**, Y. Li

CATL **361.** Activity, XPS and STEM data of Pd/Al2O3 catalyst. **A.C. Banerjee**, M. Bozack

CATL **362.** Size-controlled NHC-stabilized Ni and Cu NPs immobilized in CNTs Application in stereoselective hydrogenation. **C. Claver**, M. Díaz de los Bernardos, S. Pérez-Rodríguez, C. Godard, S. Castillon

CATL **363.** Influence of mesoporosity in zeolites on the catalytic mechanism for the conversion of methanol to hydrocarbons. **Z. Liu**, X. Dong, Y. Han

CATL **364.** Hydrogenation of CO2 to methanol using Cu-based catalysts derived from bimetallic metal-organic framework precursor. **H. Wang**, C. Zhang, P. Gao, Y. Sun

CATL **365.** Cobalt-nitrogen-doped 3D porous carbon networks derived from animal bones as an efficient electrocatalyst for oxygen reduction reaction. **M. Dou**, D. He, W. Shao, F. Wang

CATL **366.** Multiwalled carbon nanotube/graphene oxide nanoribbon heterostructures as photocatalysts for CO2 conversion. **H. Liou**, C. Sun, L. Chen, K. Chen

CATL **367.** Efficient conjugated polymer methyl viologen electron transfer system for controlled photo-driven hydrogen evolution. **H. Lu**, S. Wang

CATL **368.** Tungsten-doped manganese dioxide for ozone removal. **Y. Yang**, P. Zhang

CATL **369.** Using tailored plasmonic photocatalysts for carbon dioxide hydrogenation. **X. Li**, X. Zhang, H. Everitt, J. Liu

CATL **370.** Enhanced charge separation and visible light photon-to-current efficiency in high-performance WO3 thin-film photoanodes. **J. Cen**, **Q. Wu**, **D. Yan**, **W. Zhang**, M. Liu, A. Orlov

CATL **371.** Synthesis of leading perovskite oxygen reaction catalysts by spray pyrolysis: A simpler and successful technique. **C.A. Sharpe**, L.R. Sharpe

CATL **372.** Synthesis and photocatalytic properties of Ni decorated CdS nanosheet. **M. Zhukovskyi**, M.K. Kuno

CATL **373.** Role of domain size and titanium dopant in nanocrystalline hematite thin films for water photolysis. **D. Yan**, J. Tao, K. Kisslinger, J. Cen, Q. Wu, A. Orlov, M. Liu

CATL **374.** Novel TiO2 nanorod-nanotube hybrid array for artificial photosynthesis. **M. Hasan**, N. Wongsrisujarit, K. Yeung

CATL **375.** Ionic compounds for electrochemical reduction of carbon dioxide. **A. Landers**, T. Hellstern, C. Hahn, T.F. Jaramillo

CATL **376.** Efficient dual-site carbon monoxide electro-catalysts via interfacial nano-engineering. **Z. Huang**, **Z. Wang**

CATL **377.** Mechanism of the photoredox catalytic radical coupling of benzyl bromides. **G. Park**, Y. You

CATL **378.** Hot electrons flux under methanol oxidation; The effect of external bias on the activity and selectivity. **S. Lee**, H. Lee, J. Park

CATL **379.** Effect of metal-nitrogen coordination on ORR electrocatalysis. **J. Rosenberg**, R. Paldi, J. Lu

CATL **380.** Photocatalytic C-H arylation reactions under visible light using chemically treated amorphous/crystalline titanium dioxide. **S. Bak**, H. Lee

CATL **381.** Photocatalytic degradation of organic pollutants in water using silver doped TiO2-coated core–shell magnetic nanocomposites. **S. Titinchi**, S. Noganta, H. Abbo

CATL **382.** Kinetic studies on asymmetric C=C hydrogenation of isophorone. **F. Shuangshuang**, **Y. Lanshan**, **W. Fangzhu**

CATL **383.** Outstanding antibacterial performance of bipyramidal anatase TiO2 with {101}-exposed facets. **K. Chan**, C. Lee, H. Chiu, J. Chen, C. Li, W. Lin

CATL **384.** Developing an industrial TiO2 coating process for ceramic tiles. **R. Muñoz**, R. Christoph, A. Hernández, S. Ventura

CATL **385.** Manganese nitrate/TEMPO/2,2-bipyridine - catalyzed selective aerobic oxidation of primary alcohols into aldehydes. **K. Lagerblom**, E. Lagerspets, A. Parviainen, T. Repo

CATL **386.** Efficient sugar release from softwoods by an integrated thermochemical and biological process. M. Hossain, T. Phung, S. Tulaphol, N. Sun, T. Prasomsri, **N. Sathitsuksanoh**

CATL **387.** Pd-PEPPSI pre-catalysts bearing PIB-support: Synthesis, characterization and applicability in Buchwald-Hartwig type amination. **J. Balogh**, A.R. Hlil, M.G. Rafique, R. Tuba, M. Al-Hashimi, H. Bazzi

CATL **388.** Study in the catalytic asymmetric synthesis of optically active organophosphate triesters. **T. Wei**, K. Nakayama

CATL **389.** Exploring CO2 reductive catalysis for square planar complexes: A theoretical investigation using nitrogen-doped carbon nanotube models. **Y. Chan**

CATL **390.** BIAN-NHC Ruthenium Complex for ring closing (RCM) and Ring Opening Metathesis Polymerization (ROMP). **A.R. Hlil**, J. Balogh, R. Tuba, M. Al-Hashimi, H.S. Bazzi

CATL **391.** Ru-Protein-Catalyst biohybrids designed for solar hydrogen production: Efforts to understand how electron transfer pathways effect photocatalytic function. **S.R. Soltau**, P.D. Dahlberg, J. Niklas, O. Poluektov, K.L. Mulfort, L.M. Utschig-Johnson

CATL **392.** Novel transition-metal-free homo-polymerization of Pyrrolo[3,2-*d*:4,5-*d*']Bisthiazole (PBTz) using turbo-Grignard for organic electronics. **S. Dey**, S. Watkins, D. Sredojevic, E. Brothers, S.Y. Al Qaradawi, H.S. Bazzi, H. Bronstein, T.J. Marks, M.J. Heeney, M. Al-Hashimi

CATL **393.** Efficient Ni(II)-LDH- and LTH-based catalysts: Synthesis, characterisation and their performance in the Heck reaction. **G. Varga**, K. Karadi, A. Kukovecz, Z. Konya, S. Muráth, P. Sipos, I. Palinko

CATL **394.** Mechanistic pathways for the hydrogenation of CO2 to formic acid by Ru(PTA)4Cl2 catalyst in water and DMSO. **R. Raju**

CATL **395.** Investigating catalyst monopoly in the copper(I)-catalyzed azide-iodoalkyne cycloaddition with automated in situ reaction monitoring technology. **R. Chung**, J. Hein

CATL **396.** Using glycerol as a reducing agent for N-Oxide reductions. J. Park, **K.J. Stowers**

CATL **397.** Development and implementation of high-pressure NMR spectroscopy for study of gas-containing catalytic reactions. **S. Knapp**, A. Brezny, C.R. Landis

CATL **398.** Experimental studies on CO2, NOX, SOX adsorbing capacity of polyaniline-based materials. J. Huang, L. Gao, L. Shan, B. Meng, D. Xu, Y. Yu, **Y. Min**

CATL **399.** Comparison of two experimental outreach kits for the discovery of inexpensive, effective catalysts for solar energy conversion. J.D. Schuttlefield Christus, **A. Leichtfuss**, **Z. Chambers**

CATL **400.** Withdrawn.

CATL **401.** Development of robust covalently-linked N-heterocyclic carbenes and silica. **A.K. Jones**, R. Maglinao, W. Cochran

CATL **402.** Transformation of a novel catalytic Zn(II) metal-organic framework into a polymorph of HKUST-1. Y. Chen, **Z. Zhang**

CATL **403.** Withdrawn.

CATL **404.** Unexpected effects of mesoporosity on the catalytic performance of ZSM-5 for the fast pyrolysis of cellulose to aromatic hydrocarbons. T.C. Hoff, D.W. Gardner, R. Thilakaratne, J. Proano-Aviles, T.W. Hansen, R.C. Brown, **J. Tessonnier**

CATL **405.** Synthesis of novel phosphine ligands with an imidazolium tether for use in biphasic reaction media. **M.E. Miller**, C.J. Parnell, R.J. Rosso

CATL **406.** Withdrawn.

CATL **407.** Chemoselective oxidation of sulfides by simple metal-salen catalyst. **Z. Bai**, X. Bao

CATL **408.** Withdrawn.

CATL **409.** Oxidation/Knoevenagel condensation reaction sequence catalyzed by a bifunctional metal organic framework. **Y. Luan**

CATL **410.** Manganese dioxide catalyst for airborne formaldehyde oxidation at room temperature. **S. Rong**, P. Zhang

CATL **411.** Highly selective synthesis of diversely functionalized 1,3- and 1,4-alcohols by Regiodivergent Epoxide Opening (REO). **F.R. Muehlhaus**, A.R. Gansaeuer

CATL **412.** Oxygen-deficient tungesten oxide as versatile and efficient hydrogenation catalyst. **G. Ruijie**, L. Pan, **J. Zou**

CATL **413.** Non-metathetic synthetic applications and mechanistic inputs of Grubbs' type Ruthenium alkylidine catalysts. **A. Bokka**

CATL **414.** Cationic ferrocenium salts for the catalytic activation of propargylic alcohols. M.J. Queensen, M. Stark, **E. Bauer**

CATL **415.** Advances in organolithium cross-coupling reactions. **D. Heijnen**, V. Hornillos, F. Tosi, J. Buter, B. Feringa

CATL **416.** Valorization of biomass derived lactones into fuels and chemicals. **M. Haider**, M. Alam, S. Gupta, A. Bohre, E. Ahmad, T.S. Khan, B. Saha

CATL **417.** Cost-effective strategy to prepare high-efficient slurry-phase hydrocracking catalysts from acid-modified bauxite. **X. Bao**, **Y. Yue**, J. Li

CATL **418.** Ammonia permselective membrane reactor for urea methanolysis to dimethyl carbonate. **G. Zeng**, Y. Sun

CATL **419.** New class of porous and metal-free electrocatalyst for oxygen reduction reaction by enhanced amide functionalization on graphene. **M. Ahmed**

CATL **420.** Synthetic strategies toward Fe-N/C electrocatalysts with abundant active sites for highly efficient oxygen reduction reaction. **S. Joo**

CATL **421.** Understanding oxygen electrocatalyst mechanism of carbon network connected ternary alloy nanoparticles synthesized via supercritical reaction. J. Cho, **G. Nam**

CATL **422.** Selectivity control of CO2 reduction products by tuning nanostructure of Cu electrodes. K. Yang, W. Ko, J. Lee, J. Nah, S. Kim, H. Lee, **M. Lee**, K. Nam

CATL **423.** Withdrawn.

CATL **424.** Face-to-face, oriented hybridization of polyoxometalates with N-doped carbon nanotubes for efficient water oxidation. **I. Kim**, G. Lee, S. Kim, Y. Nam

CATL **425.** Enhancing electrocatalytic activity of bifunctional Ni3Se2 for overall water splitting through etching-induced surface nanostructuring. **A.T. Swesi**, **J. Masud**, M. Nath

CATL **426.** Unraveling oxygen anion transport in nanostructured double perovskite electrodes for solid oxide fuel cells. **M. Haider**, U. Anjum, M. Agarwal, T.S. Khan

CATL **427.** Hierarchical NiMo-based 3D electrocatalysts for highly-efficient hydrogen evolution in alkaline conditions. M. Fang, **J.C. Ho**

CATL **428.** Unraveling inherent electrocatalysis of metal nanoparticles supported on a mixed conducting oxide for high-temperature fuel cell electrodes. Y. Choi, S. Cha, S. Lee, S.O. Kim, **W. Jung**

CATL **429.** Time-series study for cleavage of -O-4 linkage during lignin disassembly with copper-doped porous metal oxide catalyst in supercritical methanol. **Y. Gao**, M. Foston

CATL **430.** Highly efficient perovskite-hematite tandem cells for unassisted solar water splitting. **M. Gurudayal**, L.H. Wong, N. Mathews, M. Graetzel, J. Ager

CATL **431.** Understanding and tuning the activation of unsaturated C-C bonds over nickel intermetallic alloys. **Y. Song**, S. Laursen

CATL **432.** Functionalization of 5-hydroxymethylfurfural by selective etherification. **M.C. Allen**, W. Gramlich, T.J. Schwartz

CATL **433.** Inverse opal organometal halide perovskites. **S. Schünemann**, K. Chen, H. Tuysuz

CATL **434.** On the aerobic selective transformation of ethanol over Me-containing vanadium oxide bronzes. **J.M. Lopez-Nieto**, L. Ruiz Rodriguez, T. Blasco, E. Rodriguez-Castellon

CATL **435.** Photocatalytic hydrogen generation over mesoporous TiO2 doped with Pd and Au. **F. Guayaquil**, B. Serrano Rosales, H. de Lasa

CATL **436.** Design of photoelectrode for water splitting utilizing semiconductor hetero-junctions. J. Xiao, **Y. Li**

CATL **437.** Photocatalytic hydrogen assessment for production using black sand as semiconductor: The application in photocatalysis process. **J.E. Cabezas**

CATL **438.** Catalytic conversion of cellulose in supercritical ethanol over carbon-based solid sulfoacid catalyst. **Z. Wen**, Y. Li

CATL **439.** Bimetallic NiRh nanoparticle catalysts for fast contact time syngas production. **T.H. Gardner**, H. Ashfaq

CATL **440.** Tuning the methane activation on Mo/ZSM-5: Effect of charge on MoxCy clusters. **T.S. Khan**, S. Mishra, S. Balyan, K.K. Pant, M. Haider

CATL **441.** Ion implantation modification of the titanate nanotubes for visible light activity. **M. Hasan**, S. Ferdousi, K. Yeung

CATL **442.** Reaction pathways of Kraft lignin deploymerization to platform chemicals on molybdenum-based catalysts in supercritical ethanol. **K. Wu**, Y. Li

CATL **443.** Depolymerization of oxidized lignin catalyzed by formic acid exploits an unconventional elimination mechanism involving 3c-4e bonding: A DFT mechanistic study. **Z. Wang**

CATL **444.** Catalytic Reductive Fractionation (CRF) of lignocellulose: A process and product overview. **S. Van den Bosch**, W. Schutyser, B.F. Sels

CATL **445.** Photochemical applications of versatile carbon nitrides. **A. Montoya**, E.G. Gillan

CATL **446.** Withdrawn.
K. Stoerzinger, S. Chambers

CATL **447.** Solvation effects on MWW-2D zeolite framework for dissociation of β-O-4 linkage. **V. Jain**, N. Rai

CATL **448.** Illuminating catalysis: The photo-reduction of ketones and aldehydes using silver nanomaterials. **M. Landry**, A.H. Moores, C.J. Barrett

CATL **449.** How the reaction media affects the methane pyrolysis and dry reforming processes: Gas-phase and molten salt media. **N. Rahimi**

CATL **450.** Systematic understandings of surface reactivity of ceramics to promote C–O bond cleavage and control C=C double bond activation. **Y. He**, S. Laursen

CATL **451.** Expeditious conversion of alginic acid to furfural in Cu(II) biphasic systems using microwaves. **C. Len**, Y. Wang, F. Delbecq, R. Varma

CATL **452.** Enhance visible light photocatalytic hydrogen production of CdS/ZnS heterostructure synthesized by hydrothermal method. **J. Kundu**, D. Pradhan

CATL **453.** Withdrawn.

CATL **454.** Spectroelectrochemical photoluminescence of reactive trap states in H-treated rutile TiO2 nanowires. **R.E. Rex**, Y. Yang, F.J. Knorr, J.Z. Zhang, Y. Li, J. McHale

CATL **455.** Template-free synthesis of hierarchical zeolite Y from natural aluminosilicate minerals. J. Yang, B. Li, H. Diao, X. Bao, **H. Liu**

CATL **456.** Mechanochemical assembly through coordination cross-linking for ordered Co/C catalyst preparation. **W. Li**, Y. Guo, Y. Guo, W. Zhan, S. Dai

CATL **457.** Withdrawn.

‡ *Cooperative Cosponsorship*

CATL **458.** Unraveling structure sensitivity in phenol hydrogenaton on Pd nanostructures. **M. Haider**, S. Seshadri, S. Gupta, T.S. Khan, V. Prabhakaran

CATL **459.** Characterising Electron and Hole Localisation on Surface Modified TiO2 Photocatalysts. **M. Nolan**

CATL **460.** Facile template-free synthesis of CaFe2O4 hierarchically hollow microspheres: Applications in visible light-driven degradation of gaseous 1,2-dichlorobenzene. **Z. Yin**, **X. Li**

CATL **461.** Tunable polymeric solid acid catalysts for biomass hydrolysis and dehydration. V. Anh, S. Wickramasinghe, **X. Qian**

CATL **462.** Visible light-responsive photodegradation of rhodamine B: Enhancement of activity and reusability of chlorophyll and Mg co-modified P25 catalysts. **T. Phongamwong**, M. Chareonpanich

CATL **463.** Synthesis of dimethyl-oxa-norbornene and alternative paths from dimethylfuran to p-xylene. **L. Wang**

CATL **464.** Withdrawn.

CATL **465.** Hydrocarbon combustion in the presence of CO. **W.F. Maier**

CATL **466.** Hexose dehydration to 5-hydroxymethylfurfural by niobia solid acid catalysts in aqueous media. **M. Tapia Reche**, A. Osatiashtiani, L.J. Durndell, M. Isaacs, A.F. Lee, K. Wilson

CATL **467.** Smart responsive nanocatalysts for self-regulation of high exothermic reactions. **L. Zhang**, Z. Liu, L. Liu, X. Ju, W. Wang, R. Xie, L. Chu

CATL **468.** Withdrawn.

CATL **469.** Catalytic production of amines from (ligno)cellulosic biomass. **M. Pelckmans**, B.F. Sels

CATL **470.** First steps of the journey from homogeneous organocatalysis to tailored catalytic materials. **R. Mas-Balleste**, J.J. Alemán, J. Luis-Barrera

CATL **471.** Size and monodispersity-dependent durability and generalized dispersion power law of supported catalysts undergoing Ostwald ripening. **S. Hu**, **W. Li**

CATL **472.** Rational design and fabrication of Ti3+-doped and Ag3PO4 QDs-sensitized TiO2 for highly efficient photocatalysis and PEC water splitting. **S. Guoqiang**, **J. Zou**, L. Pan, X. Zhang

CATL **473.** Improve the catalytic performance by utilizing the synergy between metal facet and oxide support facet for enhanced catalytic performance. **Q. Zhang**

CATL **474.** Visible light photocatalysis using a commercially available iron compound. J.K. Pagano, **R. Waterman**

CATL **475.** Constructing anatase TiO2 p-n homojunction: Applications in photoelectrochemical and photocatalytic hydrogen generation. **S. Wang**, **J. Zou**, S. Li, Y. Fang, Y. Li, Y. Qin, Z. Chen, X. Zhang

CATL **476.** Withdrawn.

CATL **477.** Photo-Catalytic hydrogen production: The role of plasmonic metals in the reaction. **H. Idriss**

CATL **478.** N-heterocyclic carbene - functionalized Ru/K-Al2O3 catalysts: Preparation, surface characterization, and tunable selective hydrogenation performances. **S. Muratsugu**, J.B. Ernst, F. Wang, M. Tada, F. Glorius

CATL **479.** Single source precursor approach for the synthesis of bimetallic molybdate catalysts. **A.W. Apblett**, A.M. Moneeb, A. Alabdulrahman, A. Bagabas, C.K. Perkins

CATL **480.** Deactivation of supported Ru catalysts during the selective CO methanation (SelMeth): Separating structural and adlayer effects. **A.M. Abdel-Mageed**, D. Widmann, S.E. Olesen, I. Chorkendorff, R.J. Behm

CATL **481.** Withdrawn.

CATL **482.** Withdrawn.

CATL **483.** Multidimensional thin film hybrid electrodes with MoS2 multilayer for electrocatalytic hydrogen evolution reaction. **E. Ahn**, B.S. Kim

CATL **484.** Synthesis and characterization of WO3-ZrO2-TiO2 nanotubes as efficient photocatalyst in the degradation of paraquat dichloride. **N.A. Eleburuike**, W. Wan Abu Bakar, R. Ali

CATL **485.** Effect of Ag shell thickness on photocatalytic degradation of organic compounds using Au@Ag core-shell bimetallic nanoparticles immobilized on electrospun TiO2 nanofibers. **N. Singh**, M. Mishra, R.K. Gupta

CATL **486.** Withdrawn.

CATL **487.** Withdrawn.

CATL **488.** High temperature calcined hematite nanotubes via the Kirkendall effect for efficient photoelectrochemical water splitting. **C. Li**, **T. Wang**, **J. Gong**

CATL **489.** Kinetic and thermodynamic insights into catalytic conversion of food waste to hydroxymethylfurfural. **I. Yu**, D. Tsang

CATL **490.** Construction of CdS and oxygen-defected CdWO4 for Z-scheme hydrogen evolution under visible light. **Z. Jingwen**, **J. Zou**

CATL **491.** Enhancing phenol photo-oxidation with palladium core-shell in TiO2 on Taylor flow system. **M.T. Yilleng**, D. Rooney, H. Manyar, E. Gimba, G. Ndukwe

CATL **492.** Efficiency of Ni-nanoparticles deposited on a hierarchically porous carbon doped with nitrogen for kraft lignin hydrogenolysis in flow and batch systems. **S.M. Lama**, M. Antonietti

WEDNESDAY MORNING

Section A

Parc 55 San Francisco

Cyril Magnin III

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Photocatalysis

Cosponsored by COMP

T. Bligaard, C. M. Friend, C. Kumar, *Organizers*

F. E. Osterloh, *Presiding*

8:00 CATL **493.** Plasmonic light focusing for enhancing and controlling catalysis on non-plasmonic metal nanoparticles. **P. Christopher**, K. Li

8:30 CATL **494.** Mapping of photocatalytic processes: Kinetics and surface chemistry dictate the interfacial charge transfer at semiconductor surface. **P.V. Kamat**, C.J. Karwacki

9:00 Intermission.

9:15 CATL **495.** Porous photocatalysts for gas phase or aqueous reactions. **R. Caruso**

9:45 CATL **496.** Surface photovoltage spectroscopy as a screening tool for solar energy conversion materials and photocatalysts. **F.E. Osterloh**, Z. Zhao, M.A. De Melo Junior, Y. Guo

10:15 Intermission.

10:30 CATL **497.** Ethanol photoreaction over anatase TiO2(101) and rutile TiO2(110) single crystals. A combined STM and online mass spectrometry study. H. Katsiev, G. Harrison, A. Wilson, G. Thornton, **H. Idriss**

11:00 CATL **498.** Engineering titania nanostructure to tune and improve its photocatalytic activity. **M. Cargnello**, C. Wrasman, I. Levin, A.C. Johnston-Peck

Section B

Parc 55 San Francisco

Cyril Magnin II

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Spectroscopy & Microscopy of Photocatalytic & PEC Materials

Cosponsored by COLL, ENFL, I&EC and INOR

S. Ardo, D. Esposito, I. Sharp, *Organizers*

G. Dukovic, *Organizer, Presiding*

8:00 CATL **499.** Ultrafast optical spectroscopy of charge transfer kinetics and charge transport at electrode/electrolyte interfaces. **T. Cuk**

8:30 CATL **500.** Dynamics of photoelectrochemical water splitting on SrTiO3. **X. Chen**, D. Aschaffenburg, T. Cuk

8:45 CATL **501.** Charge transport and reaction mechanisms of inorganic photocatalytic assemblies by transient infrared and optical spectroscopy. **H.M. Frei**

9:15 CATL **502.** Understanding optical properties and photocarrier dynamics in emerging copper-based photoelectrodes. **C. Jiang**, J.K. Cooper, I. Sharp

9:30 Intermission.

9:45 CATL **503.** Imaging and quantifying the reactivity of chemical and structural perturbations on operating water oxidation photoanodes. **J. Rodriguez Lopez**, X. Zhou, B.H. Simpson

10:15 CATL **504.** Probing surface plasmon enabled resonant excitation and chemical transformation using *in situ* vibrational spectroscopy. T.E. Tesema, B. Kafle, M.G. Tadesse, **T.G. Habteyes**

10:30 CATL **505.** Nanoscale imaging of charge carrier transport in bismuth vanadate photoanodes via photoconductive atomic force microscopy. J. Eichhorn, J.K. Cooper, L. Hess, D. Larson, **I. Sharp**, **F. Toma**

10:45 CATL **506.** Charge transfer of ZrOCoII light absorber – Co3O4 catalyst assemblies coupled by molecular wires across silica separation membrane. **G. Katsoukis**, H.M. Frei

11:00 CATL **507.** Excited electron dynamics in the 1T-2H heterophase of monolayer MoS2: Time dependent density functional theory study for photo-catalytic mechanism process. **M. Choi**, D. Shin, J. Im, H. Chang, N. Park

Section C

Parc 55 San Francisco

Market Street

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

In situ Characterization Tools

Cosponsored by COMP

T. Bligaard, C. M. Friend, C. Kumar, *Organizers*

S. Meng, *Presiding*

8:00 CATL **508.** *In Situ* and *operando* electron microscopy imaging and spectroscopy of catalysts. **P.A. Crozier**

8:30 CATL **509.** Single molecule fluorescence microscopy of a single catalyst particle: Role of defects and solvents on the proton transfer processes in zeolites. **B.M. Weckhuysen**

9:00 Intermission.

9:15 CATL **510.** Frontiers of *in situ* analytical electron microscopy for energy materials. **S. Meng**, M. Chi

9:45 CATL **511.** Watching catalysts work: Using environmental transmission electron microscopy to understand nanotube growth. **E. Stach**

10:15 Intermission.

10:30 CATL **512.** Seeing is believing: Atomic-scale imaging of catalysts under reaction conditions. **I. Groot**

11:00 CATL **513.** In situ liquid imaging of catalysts in the scanning transmission electron microscope. **I. Arslan**

11:30 CATL **514.** Raman and infrared spectroscopies as in situ and operando tool to characterize catalysts at work and reactions. **M.A. Banares**

Section D

Parc 55 San Francisco

Cyril Magnin I

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Fundamental Structure-Activity Relationships: The Interface of Operando with Physical Sciences

Cosponsored by ENVR and I&EC

M. A. Banares, M. Guerrero-Perez, *Organizers*

F. Tao, *Organizer, Presiding*

8:00 CATL **515.** Real-time and imaging XAFS and related X-ray techniques for fuel cell nanoparticle catalysis. **Y. Iwasawa**

8:40 CATL **516.** Withdrawn.

9:00 CATL **517.** Catalytic EXAFS study under reaction conditions. **M. Guerrero-Perez**, E. Mikolawska, R. Lopez-Medina, E. Rojas, M.A. Banares

9:20 Intermission.

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

9:40 CATL **518.** Withdrawn.

10:00 CATL **519.** Operando spectroscopy during ethylene polymerization by supported CrOx/SiO2 catalysts: Role of promoters. A. Chakrabarti, **I.E. Wachs**

10:20 CATL **520.** Surface morphology and catalytic activity on Pt3Ni(111) surface under CO oxidation probed with ambient pressure STM. **J. Kim**, W. Park, M. Noh, S. Lee, W. Doh, Y. Jung, J. Park

Section E

Parc 55 San Francisco

Mission I

Single-Site Heterogeneous Catalysts

Mechanisms of Bond Activation

A. Hock, *Organizer, Presiding*

8:00 CATL **521.** Hydrodeoxygenation of bio-oil model molecules and reduction of nitric oxide on single atom sites. **F. Tao**

8:30 CATL **522.** Rh-based single-site catalysis in faujasite – a surprisingly complex chemistry. V. Markova, A. Govindasamy, S. Dinda, A. Genest, **N. Roesch**

8:50 CATL **523.** Methanol partial oxidation catalyzed by singly-dispersed Pd on ZnO(100). **T.S. Rahman**, T.B. Rawal, S. Hong, S. Acharya

9:10 CATL **524.** Origin of low temperature CO oxidation activity on Ir single atoms – Experimental and computational study. **Y. Lu**, X. Ma, L. Kovarik, H. Xin, A.M. Karim

9:30 Intermission.

9:40 CATL **525.** Immobilization strategies for surface-supported molecular palladium cross-coupling catalysts. **A. Marquard**, R.H. Goldsmith

10:00 CATL **526.** Mechanistic study of hydrogen reaction on single-atom catalyst. **C. Liao**, M. Tsai, K. Sasaki, W. Chen

10:20 CATL **527.** Coordinatively unsaturated Al3+ sites anchored subnanometric ruthenium catalyst for hydrogenation of aromatics. N. Tang, **Y. Cong**, Q. Shang, T. Zhang

10:40 CATL **528.** Preparation of Nanosheet ZSM-5 zeolites and their properties for catalytic cracking of hydrocarbons. **Y. Tian**, G. Li, L. Wang, X. Zhang, G. Liu

Section F

Parc 55 San Francisco

Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

Organic Oxygenates

Cosponsored by COLL and ENVR

A. Savara, S. L. Scott, *Organizers*

C. Sievers, *Organizer, Presiding*

8:00 CATL **529.** Surface reaction of biomass derived oxygenates on metal oxide catalysts. J. So, G. Foo, J. Copeland, **C. Sievers**

8:40 CATL **530.** Mechanistic studies of benzyl alcohol oxidation to probing changes to the active site in supported Au catalysts: Support effects and proton shuttling. **B.D. Chandler**, M.Y. Santos, A. Tombo, S. Luikart, C. Pursell

9:20 CATL **531.** Systematic trends in the surface chemistry of transition metals mixed with p-block elements in atomically ordered solids (ceramics and intermetallic alloys) towards unsaturated carbon-carbon bonds for olefin and aromatic production and functionalization. Y. He, Y. Song, **S. Laursen**

10:00 CATL **532.** Molecular-level insights into the mechanism and microkinetics of aqueous-phase Pt(111)-catalyzed methanol dehydrogenation. **C. Bodenschatz**, R. Getman

10:20 CATL **533.** Mechanistic analysis of oxidative ketone cleavage over supported vanadates. **J. Bond**, A. Chatzidimitriou, R. Zhu

11:00 CATL **534.** Active site cooperativity in selective sugar transformations by oxide and zeolite-based catalysts. G. Li, E. Hensen, **E. Pidko**

11:40 CATL **535.** Mechanistic and spectroscopic evidence for active site identity and reactive intermediate structures during C-O bond rupture in small oxygenates. **M.E. Witzke**, A. Almithn, C. Coonrod, M. Triezenberg, D. Hibbitts, D. Flaherty

Synthesis & Characterization of Materials for Energy Applications

Fundamental & Molecular Models for Advanced Energy Materials/Novel Architectures, Materials & Synthetic Routes

Sponsored by ANYL, Cosponsored by CATL

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

13th International Symposium on Heavy Oil Upgrading, Production & Characterization

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Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Technique Development in Interfacial Science

Sponsored by COLL, Cosponsored by CATL

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

WEDNESDAY AFTERNOON

Section A

Parc 55 San Francisco

Cyril Magnin III

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Transition Metal & Metal Oxide Catalysis

Cosponsored by COMP

T. Bligaard, C. M. Friend, C. Kumar, *Organizers*

D. J. Stacchiola, *Presiding*

1:00 CATL **536.** Well-defined transition metal-based heterogeneous catalysts: From isolated sites to atomically-precise clusters. Z.R. Jones, **S.L. Scott**

1:30 CATL **537.** Understanding CO2 reduction on transition metals. **K. Chan**

2:00 CATL **538.** Catalytic processes in oxide systems a new set of chemical descriptors. **N. Lopez**

2:30 Intermission.

2:45 CATL **539.** Utilizing machine learning to accelerate a genetic algorithm for discovery of catalysts. **P.C. Jennings**

3:15 CATL **540.** Catalysis and the nature of mixed-metal oxides at the nanometer level. **D.J. Stacchiola**

Section B

Parc 55 San Francisco

Cyril Magnin II

General Papers

S. L. Scott, *Organizer*

E. Nikolla, *Organizer, Presiding*

1:00 CATL **541.** Design and preparation of Au@MnO2 yolk-shell nanoparticles with enhanced catalytic activity for CO oxidation. **M. Gong**, C. Wang

1:20 CATL **542.** High pressure stoichiometric hydrogenation of carbon dioxide to methanol. **R. Gaikwad**, A.B. Bansode, A. Urakawa

1:40 CATL **543.** Catalytic reduction of CO2 on Bi surface: A DFT study. W. Oh, C. Rhee, J. Han, **B. Shong**

2:00 CATL **544.** Water and CO2 activation at surface modified TiO2 composites. **M. Nolan**, S. Rhatigan, W. Daly

2:20 CATL **545.** Understanding kinetics and selectivity of NiZn bimetallic catalysts for hydrogen evolution via dehydrogenation of methylcyclohexane to toluene. **L. Cavallo**, A. Jedidi

2:40 CATL **546.** Room temperature reversible electrocatalytic H2 oxidation/production achieved with molecular complexes containing aromatic amino acids in the outer coordination sphere. **N.P. Boralugodage**, A. Dutta, B. Ginovska, G. Buchko, M.J. O'Hagan, S. Raugei, W.J. Shaw

3:00 Intermission.

3:15 CATL **547.** Deoxygenation of coal bed methane: The structure evolution and catalytic performance of LaCoO3 perovskite catalyst. **Y. Guo**, W. Li, Y. Guo, W. Zhan

3:35 CATL **548.** Density functional theory study of the interactions of C, O, and CO with nickel surface alloys. **L.H. Sprowl**, B. Adam, J. Tucker, L. Arnadottir

3:55 CATL **549.** Kinetic consequences of oxygen and carbon in C-H bond cleavage and C-H bond formation on transition metal and alloy clusters. W. Tu, P. Lachkov, **Y. Chin**

4:15 CATL **550.** Y-doped CeO2 nanorod catalyzed oxidative dehydrogenation of cyclohexane and cyclohexene. Z. Wang, **K.J. Balkus**

4:35 CATL **551.** New insights of aldol reactions catalyzed by heterogeneous gold catalysts. **R. Ye**, D. Toste, G.A. Somorjai

Section C

Parc 55 San Francisco

Market Street

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Devices, Assemblies & Hybrid Processes

Cosponsored by COLL, ENFL, I&EC and INOR

S. Ardo, G. Dukovic, I. Sharp, *Organizers*

D. Esposito, *Organizer, Presiding*

1:00 CATL **552.** Sunlight-driven hydrogen formation by membrane-supported photoelectrochemical water splitting. **N.S. Lewis**

1:30 CATL **553.** Modelling of particle-based photoelectrochemical and photocatalytic water splitting. **S. Haussener**

2:00 CATL **554.** Withdrawn.

2:15 CATL **555.** Towards evaluating reaction kinetics in photocatalytic CO2 reduction: Influence of CO2 partial pressure and light intensity. **J. Strunk**

2:30 CATL **556.** Hybrid photo-electrochemical and photo-voltaic cells (HPEV cells). **G. Segev**, J.W. Beeman, K.A. Walckzak, J. Greenblatt, I. Sharp

2:45 Intermission.

3:00 CATL **557.** High photoelectrochemical water splitting efficiencies: Materials development and measurement challenges. **J.A. Turner**, T.G. Deutsch, J. Young, H. Doescher, M. Steiner

3:30 CATL **558.** Development of solar fuels photoanodes through combinatorial integration of Ni-La-Co-Ce oxide and Ni-Fe-Co-Ce oxide catalysts on BiVO4. **J. Haber**, D. Guevarra, A. Shinde, L. Zhou, G. Li, G. Liu, **I. Sharp**, J. Neaton, F. Toma, J. Gregoire

3:45 CATL **559.** Efficient spontaneous water splitting using solid-state Z-scheme photocatalyst sheet. **Y. Li**, Q. Wang, T. Hisatomi, I. Sharp, K. Domen

4:00 CATL **560.** Nanostructured tandem Si-Ta3N5 photoanodes for solar water splitting. **I. Narkeviciute**, P. Chakthranont, A. Mackus, C. Hahn, B. Pinaud, S.F. Bent, T.F. Jaramillo

4:15 CATL **561.** Enhanced visible-light driven antibiotic activity of graphitic carbon nitride (g-C3N4) films derived from urea. **J.H. Thurston**, K. Cornell, N.M. Hunter

4:30 CATL **562.** Tailoring the semiconductor interface for energetic tuning and improved stability purposes. **J. Gu**

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Section D

Parc 55 San Francisco

Cyril Magnin I

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Fundamental Structure-Activity Relationships: The Interface of Operando with Physical Sciences

Cosponsored by ENVR and I&EC

M. A. Banares, F. Tao, *Organizers*

M. Guerrero-Perez, *Organizer, Presiding*

1:00 CATL **563.** Power of oxide-metal interfaces: *In-situ* studies of the water-gas-shift reaction. **D.J. Stacchiola**

1:40 CATL **564.** Inelastic neutron studies of ethanol interaction with transition aluminas. **J.Z. Larese**, S. Adak, C.A. Crain, N. Strange, C. Sumner

2:00 Intermission.

2:20 CATL **565.** Combined operando x-ray diffraction/Raman spectroscopy of catalytic solids in the laboratory: The Fischer–Tropsch synthesis catalyst showcase. **B.M. Weckhuysen**

3:00 CATL **567.** *Operando* Raman-MS spectroscopy during ethylene oxidation by supported Ag/Al2O3 catalysts. J. Jehng, M.E. Ford, **I.E. Wachs**

Section E

Parc 55 San Francisco

Mission I

Single-Site Heterogeneous Catalysts

Mechanisms of Bond Activation

A. Hock, *Organizer, Presiding*

1:00 CATL **568.** Low-temperature C4 dehydrogenation at ionic Cu sites in beta zeolite to enable C4 recycle in dimethyl ether homologation. **C.A. Farberow**, S. Cheah, S. Kim, J. Miller, J.R. Gallagher, J. Hensley, J. Schaidle, D.A. Ruddy

1:20 CATL **569.** AIM-ing for single-site heterogeneous catalysts for gas-phase chemical transformations. Z. Li, N. Schweitzer, O.K. Farha, **J.T. Hupp**

1:50 CATL **570.** Investigation of surface alkylation strategy in Surface Organometallic Chemistry (SOMC): In Situ generation of a silica-supported niobium methyl catalyst for ethylene oligomerization. **A. Hamieh**, R. Dey, M. Samanatary, Y. Chen, b. nekoueishahraki, J. Basset

2:10 CATL **571.** Supported single-site d0 organozirconium complexes for (stereo) selective catalysis. **M. Stalzer**, C.P. Nicholas, M. Delferro, T.J. Marks

2:30 CATL **572.** Single site tetra-coordinated aluminium hydride supported on mesoporous silica. From dream to reality! **B. Werghi**, J.M. Basset

2:50 CATL **573.** Trends of SiO2 supported single-site catalysts for alkene hydrogenation based on combined DFT and experimental studies. **C. Liu**, J. Camacho-Bunquin, M. Ferrandon, M. Delferro

3:10 Intermission.

3:20 CATL **574.** Understanding site isolation of Pd and Ni in Zn-based bulk intermetallics during the selective hydrogenation of alkynes. A. Dasgupta, G. Kumar, H. He, M.J. Janik, **R.M. Rioux**

3:50 CATL **575.** Mechanistic study of ethene dimerization on isolated nickel cations confined within molecular sieves. **R. Joshi**, R. Gounder

4:10 CATL **576.** Surface Organometallic Chemistry (SOMC): The effects of tethering highly reactive catalysts to well defined silica supports. **M.J. Kelly**

4:30 CATL **577.** In-situ shape control of polyolefins products by the design of the catalyst supports. **M. Klapper**, D. Vidakovic, A.A. Alsaygh, I. Freudensprung, K. Muellen

4:50 CATL **578.** Supported single-site organochromium catalysts for the production of high performance polyethylene materials. **M. Enders**

Section F

Parc 55 San Francisco

Mission II/III

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms: Hydrogenation

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

1:00 CATL **579.** Determining the active site for selective C=O bond hydrogenation: Understanding the role of the Pt–support interface. **L. Baker**, Y. Mueanngern, X. Yang

1:40 CATL **580.** Elucidating the mechanism of the Lewis acid catalyzed production of 1,3-butadiene from ethanol with modulated DRIFTS-MS. P. Mueller, S.P. Burt, A.M. Love, W.P. McDermott, P. Wolf, **I. Hermans**

2:20 CATL **581.** Withdrawn.

3:00 Intermission.

3:20 CATL **582.** Mechanistic investigation and development of new catalytic routes for the zeolite catalyzed hydrocarbon conversion processes as aided by operando spectroscopy. **A. Dutta Chowdhury**, K. Houben, M. Baldus, B. M. Weckhuysen

3:40 CATL **583.** Mechanistic studies on the hydrogenation of CO2 to methanol: Importance of metal-oxide interfaces in the activation of CO2. **J. Rodriguez**, P. Liu, S.D. Senanayake, D.J. Stacchiola

4:00 CATL **584.** Computational intermediates identification and structure dependence of chain growth mechanism and product selectivity in Fischer-Tropsch synthesis on Co catalysts. **H. Su**

4:20 CATL **585.** Kinetics and thermodynamics of surface reactions involved in the deactivation of Fischer-Trospsch catalysts. **M. Corral Valero**, P. Raybaud

Synthesis & Characterization of Materials for Energy Applications

Novel Architectures, Materials & Synthetic Routes

Sponsored by ANYL, Cosponsored by CATL

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

13th International Symposium on Heavy Oil Upgrading, Production & Characterization

Sponsored by ENFL, Cosponsored by CATL

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Electrons & Photons in Interfacial Science

Sponsored by COLL, Cosponsored by CATL

State-of-the-Art Methods for Modeling Materials Chemistry

Sponsored by COMP, Cosponsored by CATL and MPPG‡

THURSDAY MORNING

Section A

Parc 55 San Francisco

Cyril Magnin III

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Biomass Catalysis

Cosponsored by COMP

T. Bligaard, C. M. Friend, C. Kumar, *Organizers*

L. Grabow, *Presiding*

8:00 CATL **586.** Design of catalysts for the conversion of biomass to fuels and lubricants. **A.T. Bell**

8:30 CATL **587.** Mechanisms of catalytic conversion and upgrading of lignin first to value added chemicals. **M.M. Abu-Omar**, H. Luo, I. Klein

9:00 Intermission.

9:15 CATL **588.** Computational design of dual site catalysts for hydrogen-efficient hydrodeoxygenation of bio-oil compounds. S. Kasiraju, J. Arce-Ramos, B. Baek, **L. Grabow**

9:45 CATL **589.** Catalytic conversion of lignin models and extracts into oxygenates. N. Luo, M. Wang, T. Hou, C. Zhang, H. Li, **F. Wang**

10:15 Intermission.

10:30 CATL **590.** Tuning the activity and selectivity of metal oxide catalysts with organic monolayers. **J.W. Medlin**, L. Ellis, D.K. Schwartz

11:00 CATL **591.** Catalytic reductive fractionation of lignocellulose: Introducing the lignin-first biorefinery. T. Renders, W. Schutyser, S. Van den Bosch, S. Koelewijn, **B. Sels**

Section C

Parc 55 San Francisco

Market Street

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Engineering Operando to Larger Scale: Shaped Catalysts & Process Control

Cosponsored by ENVR and I&EC

M. A. Banares, M. Guerrero-Perez, F. Tao, *Organizers*

B. M. Weckhuysen, *Presiding*

8:00 CATL **592.** Reaction mechanism for SCR of NO with NH3 by supported V2O5-WO3/TiO2 catalysts. M. Zhu, M.E. Ford, U. Tumuluri, Z. Wu, **I.E. Wachs**

8:40 CATL **593.** Operando spectroscopy and DFT studies for assessment of mechanistic phenomena on ammonia reduced NO by vanadia SCR. **S.B. Rasmussen**, L. Arnarson, M. Daturi, P. Bazin, R. Portela, H. Falsig, P.G. Moses, **M.A. Banares**

9:00 Intermission.

9:20 CATL **594.** Operando Raman-FTIR study of gold catalysts supported on titania and ceria for VOC-related odor elimination. **Q. Wang**, P. Avila, M.A. Banares, K. Yeung

9:40 CATL **595.** Integration of operando studies of catalyst surface during catalysis and DFT calculations for mechanistic understanding at a molecular level. **F. Tao**

10:00 CATL **596.** Determining the mechanism of multistep catalytic reactions with high spatial resolution operando IR and X-ray microspectroscopy measurements. **E. Gross**

Section D

Parc 55 San Francisco

Cyril Magnin I

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms: Metals

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

8:00 CATL **597.** Aluminum nitride hydrolysis enabled by hydroxyl-mediated surface proton hopping. **C. Bartel**, C. Muhich, A.W. Weimer, C. Musgrave

8:20 CATL **598.** Surface plasmon resonance spectroscopy as a platform for characterization of nanometal catalyzed cross-coupling reactions. **A. Dadgar**

8:40 CATL **599.** Withdrawn.

9:00 Intermission.

9:20 CATL **600.** Size Controlled Co Nanoparticles for Fischer-Tropsch Synthesis: Transient Kinetics for Mechanistic Insight. **W. Ralston**, G. Melaet, T. Saephan, G.A. Somorjai

9:40 CATL **601.** Borated Pt subnanoclusters on metal oxides: Coke prevention via minimizing dehydrogenation of alkenes and C-sticking. **M. Ha**, E.T. Baxter, J. Dadras, E. Jimenez-Izal, **S.L. Anderson**, A. Alexandrova

10:00 CATL **602.** Oxygen activated ultra-fast palladium nanoparticle catalyzed cross-coupling of organolithium reagents: A mechanistic insight. **F. Tosi**, D. Heijnen, B. Feringa

10:20 Intermission.

10:40 CATL **603.** Selective, stable and active Ni-based catalysts for low temperature alkene dimerization. **I. Agirrezabal-Telleria**, E. Iglesia

11:00 CATL **604.** Understanding the role of the second metal element in Pt-alloy catalysts for propane dehydrogenation. **Z. Zhao**, S. Zha, J. Gong

11:20 CATL **605.** Understanding the structures and reaction mechanism of the metal nanoparticle encapsulated UiO-66(-NH2). **D. Chen**, P. Yang, F. Zhang, F. Wang, Q. Xiao

11:40 CATL **606.** Atomic control of intermetallic surfaces towards chemoselective hydrogenation of nitroarenes to functionalized anilines. **Y. Pei**, **T. Goh**, **R. Maligal Ganesh**, **X. Li**, **Z. Qi**, **C. Xiao**, **W. Huang**

Section E

Parc 55 San Francisco

Mission I

Elucidation of Mechanisms & Kinetics on Surfaces

Oxides

Cosponsored by COLL and ENVR

A. Savara, S. L. Scott, *Organizers*

C. Sievers, *Organizer, Presiding*

8:00 CATL **607.** DFT insight into the Mars-van-Krevelen mechanism of anaerobic and aerobic reaction of polyoxometalates. **I. Efremenko**

8:20 CATL **608.** Structure-function relationships for supported copper oxide catalysts for alkane oxidative dehydrogenation. **S. Nauert**, J.M. Notestein

8:40 CATL **609.** Catalytic degradation of malachite green on binary ZnO-La2O3: Thermodynamics, kinetics and mechanism. **J. Thomforde**, A. Chaparadza

9:00 Intermission.

9:20 CATL **610.** Formaldehyde oxidation mechanism on Au-doped CeO2: A DFT study. **J. Meizan**, W. Song, J. Liu

9:40 CATL **611.** Influence of surface defects on copper oxidation via coordinated *in situ* ETEM and atomistic simulation methods. **M. Curnan**, C.M. Andolina, Q. Zhu, J. Yang, W. Al-Saidi

10:00 CATL **612.** Unraveling the catalytic origin of NbOPO4 catalyst in biomass conversion by density functional theory. **Z. Chen**, H. Wang, P. Hu

10:20 CATL **613.** Ethanol gas sensing mechanism of PdO nanoflake thin film at temperatures below 250oC. **I. Cheng**, J. Wang, C. Tsai, Y. Chen, F. Pan

Section F

Parc 55 San Francisco

Mission II/III

Single-Site Heterogeneous Catalysts

Computational & Spectroscopic Study of Single Atom Sites

A. Hock, *Organizer, Presiding*

8:00 CATL **614.** Boron nitride nanomesh: a robust template for monodisperse oxide cluster adsorption. M. Müllner, J. Balajka, A. Hemmi, M. Schmid, U. Diebold, **S. Mertens**

8:20 CATL **615.** Growth and stability of titanium oxide nanoclusters on graphene/Ru(0001). **R.T. Frederick**, Z. Novotny, F. Netzer, G.S. Herman, Z. Dohnalek

8:40 CATL **616.** Withdrawn.

9:00 CATL **617.** Selective Oxidation of Benzyl Alcohol to Benzaldehyde by manganese oxide nanoparticles as catalyst. **K.A. Omer**

9:20 Intermission.

9:30 CATL **618.** Polyoxometalates as single site catalysts: Evidence for proton cluster synergy. **T.J. Wilke**, M.A. Barteau

9:50 CATL **619.** Preparation, structure, and surface chemistry of Ni-Au single atom alloys. **Z. Wang**, M. Darby, A. Therrien, **M. El Soda**, A. Michaelides, M. Stamatakis, E.H. Sykes

10:10 CATL **620.** PtNi/NiO Clusters coated by small sized hollow sillica: Novel design for efficient catalytic hydrogen production from hydrolysis of ammonia–borane. **G. Yuzhen**, R. Lu

10:30 CATL **621.** Tailored design of Pd catalyst supported on chemically modified silica hollow microspheres with penetrating macroporous shells for NBR hydrogenation. **J. Chen**, T. Cheng, A. Cai, Z. Wu, H. Liu, P. Yuan

Functional Porous Materials for Sustainable Energy

Sponsored by ENFL, Cosponsored by CATL and MPPG‡

13th International Symposium on Heavy Oil Upgrading, Production & Characterization

Sponsored by ENFL, Cosponsored by CATL

THURSDAY AFTERNOON

Section A

Parc 55 San Francisco

Cyril Magnin III

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Machine Learning Tools for Catalyst Genome

Cosponsored by COMP

T. Bligaard, C. M. Friend, C. Kumar, *Organizers*

J. Hachmann, *Presiding*

1:00 CATL **622.** Automated materials property prediction using thermodynamic density of states and machine learning. **S. Curtarolo**, C. Toher

1:30 CATL **623.** Statistical learning aided design of catalyst chemistry. **K. Rajan**

2:00 Intermission.

2:15 CATL **624.** Data-driven *in silico* tools for the rational design of catalytic systems and the exploration of chemical space. **J. Hachmann**

2:45 CATL **625.** Open-source tools for generating and analyzing large materials data sets: FireWorks, MatMethods, and MatMiner. **A. Jain**

3:15 Intermission.

3:30 CATL **626.** Quantum machine learning. **O. von Lilienfeld**

4:00 CATL **627.** Dark reactions project: A machine learning approach to materials discovery. **A.J. Norquist**, J. Schrier, S. Friedler

Section B

Parc 55 San Francisco

Cyril Magnin II

General Papers

S. L. Scott, *Organizer*

E. Nikolla, *Organizer, Presiding*

1:00 CATL **628.** Catalytic reaction study via strong metal-support interactions of nanocatalysts. **K. An**

1:20 CATL **629.** Characterization of soft-templated mesoporous zeolites: Techniques and insights. **J. Obrien**, S.L. Kobaslija, S. Fernandez, M. Ostraat

1:40 CATL **630.** Titanium-based organic frameworks for chemical transformations. **S. Verma**, R.S. Varma

2:00 CATL **631.** Metal organic frameworks and their catalysis applications in water. **M.M. Reynolds**, M. Neufeld, H. Rubin

2:20 CATL **632.** Comparative characterization of catalytic properties of colloidal and supported gold nanoparticle catalysts by ligand adsorption method. **S. Chakraborty**, S.M. Ansar, C.L. Kitchens

2:40 Intermission.

2:55 CATL **633.** Withdrawn.

3:15 CATL **634.** Palladium(II)-catalyzed directed anti-hydrochlorination of unactivated alkynes with *In Situ* generated HCl. **A.L. Cantu**, J. Derosa, K. Engle

3:35 CATL **635.** Co-Catalyst of layered oxide and spinel for NOx reduction to N2 through N2O. **M.P. Rowe**, T.C. Peck, M. Jones

3:55 CATL **636.** Direct synthesis of hydrogen peroxide from hydrogen and oxygen over a Palladium-based bimetallic heterogeneous catalyst. **C. Zhang**

4:15 CATL **637.** Implicit and explicit solvation models for computing free energies of activation and reactions at solid-liquid interfaces. **M. Saleheen**, A. Heyden

4:35 CATL **638.** Enhanced activity of Ce-incorporated MOR in DME carbonylation through tailoring the distribution of Brønsted acid. **S. Huang**, Y. Li, X. Ma, S. Wang, Z. Yujun

4:55 CATL **639.** Copper-Catalyzed hydroamination of alkynes and allenes. Scope and mechanism studies. **F. Monnier**

Section C

Parc 55 San Francisco

Market Street

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Engineering Operando to Larger Scale: Shaped Catalysts & Process Control

Cosponsored by ENVR and I&EC

M. A. Banares, M. Guerrero-Perez, F. Tao, *Organizers*

D. J. Stacchiola, *Presiding*

1:00 CATL **640.** Identification of sulfur atoms as catalytically active sites for proton reduction on amorphous molybdenum sulfide. **B. Yeo**

1:40 CATL **641.** Withdrawn.

2:00 CATL **642.** Low-temperature methane combustion over Pd/H-ZSM-5: Active Pd sites with specific electronic properties modulated by acidic sites of H-ZSM-5. **Y. Guo**, W. Li, Y. Guo, W. Zhan

2:20 CATL **643.** Withdrawn.

Section D

Parc 55 San Francisco

Cyril Magnin I

Elucidation of Mechanisms & Kinetics on Surfaces

Oxidation Reactions

Cosponsored by COLL and ENVR

S. L. Scott, C. Sievers, *Organizers*

A. Savara, *Organizer, Presiding*

1:00 CATL **644.** Quantitative spectroscopic analysis of the role of oxy-carbon surface species in the mechanism of propane oxidation over Pt/Al2O3. **C. O'Brien**, I. Lee

1:40 CATL **645.** Kinetic and spectroscopic evidence for periodic trends in olefin epoxidation over group IV and V *BEA. **D. Bregante**, P. Priyadarshini, D. Flaherty

2:00 CATL **646.** Tuning carbon monoxide preferential oxidation properties on platinum alloy nanoparticle catalyst via engineering the active sites. **Z. Peng**, S. Hwang, Y. Pan, X. Shen, E. Yurchekfrodl

2:20 CATL **647.** Adsorption and decomposition of dimethyl methylphosphonate on metal oxide surfaces under atmospheric conditions. **A.R. Head**, L. Trotochaud, R. Tsyshevsky, Y. Yu, O. Karslioglu, M. Kukla, H. Bluhm

3:00 Intermission.

3:20 CATL **648.** Control of metal-oxide interfaces for ceria-based nanocatalysts. **S. Lee**, J. Seo, W. Jung

3:40 CATL **649.** Unprecedented CO oxidation performance of Pd/CeO2 prepared by flame spray pyrolysis. **G. Spezzati**, Y. Su, J. Hofmann, E. Hensen

4:00 CATL **650.** Withdrawn.

4:20 CATL **651.** Mechanistic studies of H2 oxidation to understand the role of water in CO PROx. **T. Whittaker**, J. Saavedra, C. Pursell, B.D. Chandler

Section E

Parc 55 San Francisco

Mission I

Elucidation of Mechanisms & Kinetics on Surfaces

Beyond Hydrocarbons

Cosponsored by COLL and ENVR

A. Savara, S. L. Scott, *Organizers*

C. Sievers, *Organizer, Presiding*

1:00 CATL **652.** Quantitative assessment of the role of dissolved oxygen in catalytic reduction of 4-nitrophenol. **E. Menumerov**, R.A. Hughes, S. Neretina

1:20 CATL **653.** Competitive adsorption of sulfur compounds in diesel on corner sites of Ni-Mo-S, Co-Mo-S and MoS2 nanocluster - A mechanism study based on DFT calculations. **S. Ding**, Y. Zhou, Q. Wei

1:40 CATL **654.** Gallium modified USY zeolites as an effective co-support for ultra deep hydrodesufurization catalysts on inferior diesels-its high isomerization selectivity. **W. Zhou**, Y. Zhou, Q. Wei

2:00 Intermission.

2:20 CATL **655.** NH3-SCR Mechanism on Cu-SAPO-18 catalysts: A DFT+U study. **J. Deng**, W. Song, Z. Zhao, L. Zhao, J. Liu

2:40 CATL **656.** Mechanistic study of selective catalytic reduction of NOx with NH3 over Mn-TiO2: A combination of experimental and DFT study. **H. Zheng**, W. Song, J. Liu, Z. Zhao

‡*Cooperative Cosponsorship*

3:00 CATL **657.** Cu-catalyzed etching of graphene layers through carbon hydrogenation. **G. Cheng**, I.G. Calizo, A.R. Hight Walker

3:20 CATL **658.** Distinctive catalysis of supported Pt and Au nanoparticles in aerobic oxidation of polyols. **B. Xu**, S. Liu, Z. Yuan

CELL

Division of Cellulose and Renewable Materials

M. Roman, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Chemistry of Cellulosic Natural Products (see *AGFD*, Wed)

Carbohydrate-Based Hybrid Materials for Nanomedicine (see *CARB*, Mon, Tue)

Carbohydrate-Based Nanomaterials & Drug-Delivery Vehicles (see *CARB*, Wed)

LPS: Chemistry, Synthesis & Applications (see *CARB,* Tue)

Biomass & Biofuel Processing (see *ENFL,* Tue, Wed)

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications (see *PMSE,* Tue, Wed, Thu)

SOCIAL EVENTS:

CELL Awards Banquet, 6:00 PM: Tue

BUSINESS MEETINGS:

Governance Meeting, 5:30 PM: Wed

Technical Program Meeting, 7:00 PM: Wed

Executive Committee Meeting, 5:00 PM: Sat

SUNDAY MORNING

Section A

Moscone Center

252/260

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Drug Delivery

Cosponsored by CARB

Financially supported by EPNOE, Eastman Chemical Company, VT Fralin Life Science Institute, VT College of Natural Resources and Environment, VT Department of Sustainable Biomaterials, Carbohydrate Polymers (Elsevier)

P. E. Fardim, O. J. Rojas, *Organizers*

C. M. Buchanan, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **1.** Polysaccharides in drug delivery: An overview. **M.F. Wempe**

8:30 CELL **2.** Polyscaccharides in drug delivery: Applications of cellulose derivatives for oral drug delivery. **G. Ilevbare-Okoh**

8:55 CELL **3.** From computational modelling towards mechanistic design of polymers for oral drug delivery. **L.I. Mosquera-Giraldo**, C.H. Borca, X. Meng, Y. Dong, K.J. Edgar, L.V. Slipchenko, L. Taylor

9:20 CELL **4.** Withdrawn.

9:45 Intermission.

10:00 CELL **5.** Cellulose nanocrystal conjugates for drug delivery and bioimaging applications. **M. Roman**

10:25 CELL **6.** Supramolecular design of cellulose hydrogel microspheres. **P.E. Fardim**, P. Trivedi, J. Schaller, J. Gustafsson

10:50 CELL **7.** Immunosensor based on cellulose nanofibrils for C-reactive protein detection. Y. Zhang, **O.J. Rojas**

11:15 CELL **8.** Self assembly of *A. Tequilana* fructans and encapsulation of ibuprofen for targeting oral drugs to the colon. **G. Toriz Gonzalez**, C. Miramontes-Corona, J. Ferrer, A. Escalante, E. Delgado, R.I. Corona-Gonzalez, A. Soltero

Section B

Moscone Center

262

Processing & Properties of Biobased Composites & Blends

Financially supported by EPNOE

J. R. Barone, P. R. Navard, *Organizers*, *Presiding*

8:05 CELL **9.** Effect of ethylene glycol-water mixed solvent on the synthesis of iron oxide/carbon nanocomposites and their adsorption performance. **S. Liu**

8:30 CELL **10.** Solvent-exchanged porous bacterial cellulose nanopaper as reinforcement for polymers. **A. Santmarti**, M. Hervy, K. Lee

8:55 CELL **11.** Water-based dissolution of wood cellulose and design of novel cellulose-based nanocomposite materials. **M. Norgren**, J. Yang, C. Costa, A. Eivazihollagh, F. Carlsson, C. Dahlström, B. Medronho, H. Edlund, B. Lindman

9:20 CELL **12.** Facile Method for the Suspension, Dispersion, and Fabrication of Cellulose-based Plastics. D.H. White, C.J. Huntley, **M.L. Curry**

9:45 Intermission.

10:00 CELL **13.** Cellulose/vaterite nanocomposites: Sonochemical synthesis, and their applications in drug delivery and protein adsorption. **L. Fu**, M. Ma, F. Xu, X. Zhang

10:25 CELL **14.** Simple synthesis method towards amino-functionalized carbon dots: Carbonization of chitosan. **X. Liu**, J. Pang, F. Xu, X. Zhang

10:50 CELL **15.** Synthesis and characterization of hydroxypropyl methylcellulose/xyloglucan blend films for release of gentamicin drug. **S. Kondaveeti**

11:15 CELL **16.** How can a single methyl group drastically modify the microstructure of a biocomposite and affect its mechanical properties? **A. Gallos**, J. Beaugrand, G. Paes, **F. Allais**

Section C

Moscone Center

270

Cellulose Structure & Biosynthesis

In the Plant Cell Wall

Cosponsored by BIOL, BIOT, CARB and ENFL

Financially supported by Department of Energy - Office of Science

P. Langan, H. M. ONeill, J. Zimmer, *Organizers*

N. Carpita, D. Cosgrove, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **17.** 3D Nano-architecture and mechanical properties of *Arabidopsis thaliana* plant cell walls by cryo-electron tomography of vitreous sections. **M. Auer**

8:30 CELL **18.** Visualizing cellulose microfibril movements during stress-induced and endoglucanase-induced extensions of plant primary cell walls. **D. Cosgrove**

8:55 CELL **19.** Advances in combining neutron scattering with molecular simulations to understand cell wall structure. **P. Langan**, B. Evans, H.M. ONeill, R. Shah, S. Pingali, V. Urban, D. Sawada, J. Smith, L. Petridis, D. Vural, B.H. Davison

9:20 CELL **20.** Microfibril orientation, spacing and bundling in secondary cell walls: Implications for catalytic deconstruction. **B.S. Donohoe**, J.D. HInkle, P.N. Ciesielski, M.F. Crowley, N.S. Mosier, C. Chapple, M. Himmel

9:45 Intermission.

10:00 CELL **21.** Polymorphic structures and pectin interactions of cellulose in primary plant cell walls from multidimensional solid-state NMR. T. Wang, P. Phyo, H. Yang, S. Kiemle, D. Cosgrove, J.D. Kubicki, **M. Hong**

10:25 CELL **22.** Mesoscale order of cellulose microfibrils in plant cell walls: Sum Frequency Generation (SFG) vibrational spectroscopy study. **S.H. Kim**

10:50 CELL **23.** Density functional theory modeling of cellulose polymer assembly. **J.D. Kubicki**, H. Watts, H. Yang, D. Oehme, L. Petridis, Y.G. Yingling

11:15 CELL **24.** Impact of alterations in lignin deposition on cellulose organization of the plant cell wall. J. Liu, J. Kim, J. Cusumano, C. Chapple, **L. Makowski**

Section D

Moscone Center

272

Nanocellulose Processing & Analysis

Novel Processes

Cosponsored by AGFD, ANYL, CHAS and I&EC

Financially supported by TAPPI

W. Y. Hamad, T. Lindström, M. Roman, *Organizers*

M. Bortner, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **25.** Deep eutectic solvents in nanocellulose production. **J.A. Sirviö**, M. Visanko, T. Selkälä, H. Liimatainen

8:30 CELL **26.** Ionic liquid-cellulose-in-oil microemulsions: Molecular weight dependence and directed morphology of cellulose nanoparticles. **J.R. Alston**, N. Redeker, M. Khan, J.M. Mabry

8:55 CELL **27.** Imidazole: A new tunable reagent for producing nanocellulose. **J. Mao**, H. Abushammala, H. Hettegger, T. Rosenau, M. Laborie

9:20 CELL **28.** One pot generation of hydrophobic nanocellulose by a multi-functional agent. **J.Y. Fukuda**

9:45 Intermission.

10:00 CELL **29.** Cellulose nanostructure obtained by enzymatic hydrolysis: The effects of treatment time. **D. Rosa**, C. Bauli, D. Rocha

10:25 CELL **30.** Investigation of surface interactions of micro/nano-cellulose with metal ions at micro-nano-molecular scale. **C. Zhu**, A. Mathew

10:50 CELL **31.** Phosphated cellulose nanocrystas: Isolation and bioengineering applications. **S. Camarero-Espinosa**, T. Kuhnt, B. Rothen-Rutishauser, J. Foster, C. Weder

11:15 CELL **32.** Development of the continuous production process Kyoto process of CNF reinforced plastics. **H. Yano**, F. Nakatsubo, T. Semba, K. Kitagawa

11:40 Concluding Remarks.

Section E

Moscone Center

274

New Horizons in Sustainable Materials

Renewable Polymers: Isolation, Structure & Properties

Cosponsored by POLY

M. G. Laborie, S. H. Renneckar, N. Robitaille Brown, *Organizers*

N. Sathitsuksanoh, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **33.** Plant oil-based acrylic monomers for free radical polymerization. **Z. Demchuk**, I. Tarnavchyk, O. Shevchuk, V. Kirianchuk, A.S. Voronov

8:30 CELL **34.** Emulsion copolymerization of vinyl acetate with hydrophobic plant oil-based monomers: Effect of plant oil unsaturation of reaction kinetics. **K. Kingsley**, O. Shevchuk, I. Tarnavchyk, A. Voronov

8:55 CELL **35.** Random copolymerization of lactones and hydroxyacid bioaromatics using one-pot Ring Opening Polymerization (ROP) polycondensation method. **H. Nguyen**, G. Short, P. Qi, S.A. Miller

9:20 CELL **36.** Water pre- and post-hydrolysis of birch wood to produce high-purity cellulose and xylan-based compounds for material and chemical applications. **M. Borrega**, H. Sixta

9:45 Intermission.

10:00 CELL **37.** Wood-based hemicelluloses as renewable source for functional materials. **T. Nypelo**, H. Amer, C. Laine, T. Tammelin, J. Konnerth, U. Henniges, A. Potthast, T. Rosenau

10:25 CELL **38.** Multifunctional materials based on wood derived biopolymer. **H. Zhu**, L. Yang, L. Chen

10:50 CELL **39.** Novel one step method to prepare carboxycellulose nanofibers from raw biomass and their applications in heavy metal ions remediation. **P. Sharma**, B.T. Chu, B.S. Hsiao

11:15 CELL **40.** Tertiary amine catalysts for oxidizing the unsaturated components in cellulosic pulp. **G. Afsahi**, K.J. Ruuttunen, T. Vuorinen

11:40 Concluding Remarks.

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Section F

Moscone Center
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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

J. Campos-Teran, O. J. Rojas, *Organizers*

M. L. Auad, *Organizer, Presiding*

E. A. Moura, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **41.** Development of novelty Fique textile fabrics for clothing applications. **M. Restrepo**, M.C. Amaya, J. Manrique, P. Gañán, L. Velez, R. Zuluaga Gallego, C. Castro Herazo

8:30 CELL **42.** Novel recyling process for cotton polyester blended waste textiles. **S. Haslinger**, M. Hummel, H. Sixta

8:55 CELL **43.** Nanocellulose recovery from industrial bagasse of agave tequilana. **B.C. Sulbaran**, J. Hernandez, **G. Toriz Gonzalez**, O.J. Rojas, M.A. Escalante

9:20 CELL **44.** Biocatalytic functionalization of softwood galactoglucomannan through transglycosylation and enzyme engineering. **J. Morrill**, A. Rosengren, S. Butler, H. Stålbrand

9:45 Intermission.

10:00 CELL **45.** Electrodes with nanostructures used in the electrochemical analysis of pesticides in aquifers means of organic and conventional banana production in Costa Rica. **R. Zamora**, R. Starbird

10:25 CELL **46.** Modified soy protein as encapsulate excipient in pharmaceutical applications. **M. Anaya Castro**, I. Alric, S. Fullana-Girod, V. Durrieu

10:50 CELL **47.** Incorporating cellulosic passion fruit residues into pectin edible plastics. **D.R. Munhoz**, F.K. Moreira, L.H. Mattoso

11:15 CELL **48.** Residues from agroindustry as reinforcement in foams based on PBAT/PLA blend. T.T. Freitas, R. Coiado, G. Lazo, R. Oliveira, **E.A. Moura**

SUNDAY AFTERNOON

Section A

Moscone Center
252/260

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Tissue Engineering

Cosponsored by CARB

Financially supported by EPNOE, Eastman Chemical Company, VT Fralin Life Science Institute, VT College of Natural Resources and Environment, VT Department of Sustainable Biomaterials, Carbohydrate Polymers (Elsevier)

C. M. Buchanan, O. J. Rojas, *Organizers*

P. E. Fardim, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **49.** Tubular biocellulose hydrogels act as temporarily implanted in vivo scaffolds and cause regeneration of bile duct by body own tissue. **D.O. Klemm**, F. Rauchfuss, F. Kramer, K. Petzold-Welcke, W. Fried, U. Settmacher

1:30 CELL **50.** Nano-designed polysaccharide-based constructs for tissue engineering applications. **J.F. Mano**

1:55 CELL **51.** Chemoenzymatic strategy to design alginates for tissue engineering. **G. Skjak-Brak**

2:20 CELL **52.** Manufacturing, characterization and use of substrates for regenerative medicine based on the specific properties of polysaccharide derivatives and biodegradable polymers. R. Kargl, T. Mohan, C. Nagaraj, A. Dobaj Štiglic, A. Olschewski, U. Maver, **K. Stana Kleinschek**

2:45 Intermission.

3:00 CELL **53.** Glycosaminoglycan nanostructures as mimics of the vascular endothelial glycocalyx. **M. Kipper**

3:25 CELL **54.** Polysaccharide based micro-nano structures for tissue engineering. **S.G. Kumbar**

3:50 CELL **55.** Development and characterization of biomembranes combining chitosan and natural- nanoliposomes for tissue engineering applications. **F. Cleymand**, E. Velot, P. Menu, E. Arab-Tehrany, J.F. Mano

4:15 CELL **56.** Bottom-up fabrication of hybrid polysaccharide/peptide amphiphile supramolecular multilayered biomaterials by combining self-assembly and layer-by-layer assembly approaches. **J. Borges**, M.P. Sousa, G. Cinar, S. Caridade, M.O. Guler, J.F. Mano

Section B

Moscone Center
262

Processing & Properties of Biobased Composites & Blends

Financially supported by EPNOE

J. R. Barone, P. R. Navard, *Organizers*, *Presiding*

1:05 CELL **57.** Role of non-cellulosic components on the microstructure and physical properties of natural fibres and their biocomposites. **N. Le Moigne**, J. Acéra Fernandez, A. Caro-bretelle, R. El Hage, A. Le Duc, M. Lozachmeur, P. Bono, A. Bergeret

1:30 CELL **58.** Influence of biochemical and histological characteristics on the properties of miscanthus-polypropylene composites. **J. Girones**, L. Vo, E. Gineau, G. Mouille, S. Arnoult, C. Lapierre, M. Brancourt, P.R. Navard

1:55 CELL **59.** Lignin- polyvinyl alcohol photo-cured composite films. Effect of lignin and UV curing agent quantity on the mechanical, optical and chemical properties. **A. Suarez**, L.Y. Perez

2:20 CELL **60.** Challenges of utilizing different lignins and blends for carbon fibers. **M. Cho**, L. Ji, M. Karaaslan, F.K. Ko, S. Renneckar

2:45 Intermission.

3:00 CELL **61.** Molecular dynamics simulation study of moisture effects on chain mobility in hemicellulose-based bio-nanocomposites as observed by ^{13}C CP/MAS NMR relaxometry. **P. Chen**, C. Terenzi, L. Berglund, J. Wohlert

3:25 CELL **62.** What defines fiber quality in wood refining? **M. Tasooji**, C.E. Frazier

3:50 CELL **63.** Withdrawn.

4:15 CELL **64.** Treatments of cellulosic fibers to reduce the water absorption in composite reinforcement. **M. Ardanuy**, H. Ventura, J. Claramunt

Section C

Moscone Center
270

Cellulose Structure & Biosynthesis

Evolution of Synthases & Fine Structure of Microfibrils

Cosponsored by BIOL, BIOT, CARB and ENFL

Financially supported by Department of Energy - Office of Science

N. Carpita, D. Cosgrove, H. M. ONeill, J. Zimmer, *Organizers*

P. Langan, *Organizer, Presiding*

C. H. Haigler, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **65.** Evolutionary perspectives on functional differentiation of CESA proteins. **A.W. Roberts**

1:30 CELL **66.** Using animal models to study cellulose biosynthesis. **K. Nakashima**

1:55 CELL **67.** Aminoethyl cellulose in bacteria: Structure, biosynthesis, and implications. **L. Cegelski**

2:20 CELL **68.** How many twists in cellulose biosynthesis can we still expect? **U. Römling**

2:45 Intermission.

3:00 CELL **69.** Patterns in cellulose fibril formation. **M.F. Crowley**, M. Himmel, L. Bu

3:25 CELL **70.** Can an 18-chain cellulose microfibril explain the scattering/diffraction data? **Y. Nishiyama**, Y. Ogawa, T. Kuribayashi

3:50 CELL **71.** Relations between co-crystallization and multiscale hydration in celluloses isolated from plants. M.M. Oliveira, A.A. Curvelo, **C. Driemeier**

4:15 CELL **72.** Understanding the mechanical induction of macromolecular defects in cellulose nanofibrils by molecular dynamics simulation and scanning probe microscopy. **P.N. Ciesielski**, R. Wagner, V. Bharadwaj, M. Himmel, J. Killgore, M.F. Crowley

Section D

Moscone Center
272

Nanocellulose Processing & Analysis

Process Parameters

Cosponsored by AGFD, ANYL, CHAS and I&EC

Financially supported by TAPPI

M. Bortner, T. Lindström, M. Roman, *Organizers*

W. Y. Hamad, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **73.** Limiting factors for cellulose nanocrystal yield assessed via TEMPO-mediated oxidation of microcrystalline cellulose. **E. Kontturi**, R. Salminen, M. Reza, J. Peyre, T. Pääkkönen

1:30 CELL **74.** Characterization and patterning of anthraquinone functionalized cellulose nanocrystals. **A. Sulkanen**, Y. Si, G. Sun, G. Liu

1:55 CELL **75.** Surface polarity engineering of crystalline nanocellulose using a food-grade surfactant for improved sustainable biocomposites. **K. Chi**, J.M. Catchmark

2:20 CELL **76.** Microfibrillated cellulose produced with a high consistency enzymatic process. **T.C. Maloney**, K. Dimic-Misic, S. Ceccherini, J. Kuusisto, A. Suurnäkki, O. Mattila, S. Grönqvist

2:45 Intermission.

3:00 CELL **77.** Determination of hydrophobicity in amphiphilic nanocellulose imparted by Aqueous Counter Collision (ACC). **T. Kondo**, K. Tsuboi, S. Yokota

3:25 CELL **78.** Understanding cell wall longitudidal structure for producing cellulose nanofibrils by disk milling with dilute acid prehydrolysis. **J. Zhu**

3:50 CELL **79.** Cellulose fibre in situ fibrillation by twin screw extrusion. **F. Rol**, O. Nechyporchuk, B. Karakashov, N. Belgacem, J. Bras

4:15 CELL **80.** Influence of monosaccharide composition in TEMPO-mediated oxidation to produce cellulose nanofibrils from corn husk and banana rachis. **C. Gomez Hoyos**, J. Velázquez-Cock, A.M. Serpa Guerra, R. Zuluaga Gallego, C. Castro Herazo

4:40 Concluding Remarks.

Section E

Moscone Center
274

New Horizons in Sustainable Materials

Nanocellulose Materials & 3D Structures

Cosponsored by POLY

M. G. Laborie, N. Robitaille Brown, N. Sathitsuksanoh, *Organizers*

S. H. Renneckar, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **81.** Environmental effects on the organization and structure of mechanically adaptable biopolymer networks. **Z. Walsh**, L. Averous

1:30 CELL **82.** Hydrodynamic stability of reacting multilayer flows in a Hele-Shaw cell. **J. MacKenzie**

1:55 CELL **83.** 3D printing of cellulose nanocrystals and nanocomposites. **G. Siqueira**, D. Kokkinis, R. Libanori, M. Hausmann, S. Gladman, A. Neels, P. Tingaut, T. Zimmermann, J. Lewis, A. Studart

2:20 CELL **84.** Cellulose nanofibril-cell adhesive peptide conjugates for 3D bioprinted tissue models. **E. Karabulut**, A. Sousa Morais, P. Gatenholm

2:45 Intermission.

3:00 CELL **85.** Functional lignocellulosic materials: Engineering smart bio-hybrids from a natural anisotropic scaffold. **E. Cabane**, T. Keplinger, S. Kostic, M. Vidiella del Blanco, S. Vitas, Y. Wang, I. Burgert

3:25 CELL **86.** Non-proteolytically digestible micro-patterning cell scaffolds by inkjet-printing of chitinous nanocrystals. **Y. Teramoto**, S. Suzuki, T. Katsuragawa

3:50 CELL **87.** Chemical modifications for the synthesis of functional materials from sustainable nano/cellulose. **K. Zhang**

4:15 Introduction of the KINGFA Awardee.

4:20 CELL **88.** Optimizing both thermal and colloidal stability of cellulose nanocrystal through acid hydrolysis. **E.D. Cranston**, O. Vanderfleet, M.S. Reid

‡ *Cooperative Cosponsorship*

Section F

Moscone Center
276

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

M. L. Auad, O. J. Rojas, *Organizers*

J. Campos-Teran, *Organizer, Presiding*

K. A. Oksman, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **89.** Biomass conversion into functional bioplastics and gels. **U.M. Edlund**

1:30 CELL **90.** Effect of the culture medium in the production of bacterial cellulose from kombucha. J. Gutiérrez-Castañeda, M. Hernández-Guerrero, S. Revah, **J. Campos-Teran**, G. Vigueras

1:55 CELL **91.** Sugar produced from corncob pretreated with the combination of electron beam irradiation and enzymes. E.S. Pascoal, E.K. Kleingesinds, E.A. Moura, A.B. Lugão, **R.C. Rodrigues**

2:20 CELL **92.** Chromatographic purification of sugar cane bagasse alkaline extract. V. Oriez, **P. Pontalier**, J. Peydecastaing

2:45 Intermission.

3:00 CELL **93.** Energy efficient separation process of nanofibrils from biores-idues and their use in biocompos-ites. **K.A. Oksman**, L. Berglund, Y. Aitomaki

3:25 CELL **94.** Torrefaction analysis of woody biomasses from fast-growing plantations of Costa Rica. R. Moya, A. Rodríguez-Zúñiga, **A. Puente**

3:50 CELL **95.** Scaled-up production of biodegradable pectin plastics using continuous casting. L.B. Norcino, **D.R. Munhoz**, F.K. Moreira, L.H. Mattoso

4:15 CELL **96.** α-Eleostearic acid extraction by saponification of tung oil and its subsequent polymer-ization. **A. Murawski**, R. Quirino

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

SUNDAY EVENING

Section A

Moscone Center
Hall D

General Posters

M. Roman, *Organizer*

7:00 - 9:00

CELL **97.** Aminoethyl cellulose: *E. coli's* building material for a biofilm matrix. **W. Thongsomboon**, L. Cegelski

CELL **98.** From cellulose tissue papers to nanoporous membrane actua-tors. **H. Lin**, J.W. Dunlop, J. Yuan

CELL **99.** Understanding protein adsorp-tion to TEMPO-oxidized cellulose microfibrils. **S. Cobos**, B. Nemmaru, S.P. Chundawat, D. Athanasopoulos

CELL **100.** Combined steam and dry reforming of methane over nickel-based catalysts for upgrading biomass gasifica-tion-derived syngas. **E. Terrell**, C. Theegala

CELL **101.** Acetic acid as a precata-lyst to promote cellulose dissolu-tion. **Y. Hu**, **S. Acharya**, N. Abidi

CELL **102.** Molecular dynamics study of chitin crystal models in ionic liquids. **T. Uto**, K. Yamamoto, J. Kadokawa

CELL **103.** Preparation of amylose-grafted chitin nanofiber gels. **N. Egashira**, K. Yamamoto, J. Kadokawa

CELL **104.** Chemoenzymatic synthesis and gelation behavior of amylose-grafted poly(γ-glutamic acid). **T. Shouji**, J. Kadokawa, K. Yamamoto

CELL **105.** Withdrawn.

CELL **106.** Polyamide-polysiloxane-copolymers as examples for partially biobased thermoplastic elasto-mers. **M.A. Haslböck**, C. Zollfrank

CELL **107.** Antibacterial chitosan films containing quaternary ammonium salts modified nanocrystalline cellu-lose. **L. Ying**, X. Ren, G. Buschle-Diller

CELL **108.** Facile synthesis of high strength and oxygen-barrier performance of hot-water wood extract films. **G. Chen**, G. Fu, X. Qi, F. Peng, C. Yao, R. Sun

CELL **109.** Kinetics of chain scission and of total oxidative damage in the Fenton-induced degradation of cereal β-glu-can. **S. Boulos**, N. Burkhardt, L. Nystroem

CELL **110.** Drug delivery mechanism of sulfathiazole in films. **M.L. Auad**, M. Barde, M. Davis, S. Rangari

CELL **111.** 3D Porous structures based on lignin. **M.L. Auad**, I. Flipponen, T. Hinkle, C. Upp

CELL **112.** What are the ranges and basis of auxeticity in the phases of cellulose microfibrils? **A. Asamoah**

CELL **113.** Laccase-polymerization of ultrasound extracted bamboo substrates. **J. Fu**, A. Cavac-Paulo

CELL **114.** Toward development of new generation of peat granular products for waste water remediation: Reaction mechanism of peat surface with cations of heavy metals. **V.G. Goncharov**, H.J. Leopold, L. Kildyshova, **I.V. Kolomitsyn**

CELL **115.** Preparation and characterization of antibacterial films by pretreatment of dioxane from *Phyllostachys pubes-cens*. **Q.W. Li**, **G. Hui**, **R. Jun**, G. Ying

CELL **116.** High strength of biocomposite film prepared from hemicelluloses and cellulose. **R. Jun**, **G. Ying**, **Q.W. Li**, **H. Gao**

CELL **117.** Grafting of polyoxazo-line on chitin nanofiber film to form organo- and hydrogels. **J. Yoshida**, K. Yamamoto, J. Kadokawa

CELL **118.** Novel approach to achieve ther-moplastic arabinoxylan. **M.E. Borjesson**, G.J. Westman, A. Larsson, A. Ström

CELL **119.** Development and investiga-tion of a cellulose-based low adhesion coating for adhesive tapes. **S. von Gradowski**, M. Nau, M.A. Biesalski

CELL **120.** Influence of nanofibril-lation degree on nanocellulosic aerogel properties. J. Desmaison, B. Seantier, A. Dufresne, **J. Bras**

CELL **121.** Direct comparison of protein and lignocellulose fibers as reinforcements in polymer matrix composites. A.M. Davis, **L.E. Hanzly**, B.L. DeButts, J.R. Barone

CELL **122.** Technical lignins modified by hydroxymethylation for the production of high pressure laminates: Synthesis, characterization and mathematical mod-elling. M. Taverna, V.V. Nicolau, **D. Estenoz**

CELL **123.** Dimensional stability anal-ysis of flax fiber reinforced poly-propylene composites. A.M. Davis, **L.E. Hanzly**, B.L. DeButts, J.R. Barone

CELL **124.** Evaluating seafood industry waste products as valuable sources of chitin and chitosan. **B. Barnes**, P. Sharma, U. Onuchukwu, V. Volkis

CELL **125.** Mussel-inspired polysaccharide derivatives as examples of novel strong bioadhesives. **M. Petzold**, C. Zollfrank

CELL **126.** Disruption of cellu-lose fibers structure by Lytic Polysaccharide Monooxygenase (LPMO) enzymes. **A. Villares**, C. Moreau, C. Bennati-Granier, S. Garajova, B. Saake, J. Berrin, B. Cathala

CELL **127.** Easy process to cel-lulose-silica hybrid aero-gels. **A. Berkefeld**, M. Schestakow

CELL **128.** Algae-based biorefin-ery of *Chlorella vulgaris*. **G. Vaca Medina**, C. Mathieu, C. Raynaud

CELL **129.** Fabrication of CNC/glycerol thin films as substrate for electronic applications. **M. Rivera**, V. Pantojas

CELL **130.** Optimization of pheno-lics extraction from walnut shells through ultrasound treatment. **H. Han**, F. Zhang, Y. Wang, J. Jensen, M. Rakita, Q. Han, S. Janaswamy, Q. Xu

CELL **131.** Cellulose nanofiber surface functionalization for functional medical membrane applications. H. Durand, H. Le Drezen, N. Belgacem, E. Zeno, **J. Bras**

CELL **132.** Effects of catalytic fast pyrolysis derivatives on mechanical, thermal and surface properties of nanocellulose films. **R. Zhang**, N. Wilson, M.R. Nimlos, M. Himmel, P.N. Ciesielski

CELL **133.** Impact of vanillin on the rheological and phase behav-ior of Cellulose Nanocrystals (CNCs). **J. Mao**, R. Ma, M. Laborie

CELL **134.** Enhancement of PVA/MMT composite film by chitin nanowhis-kers. **Y. Guan**, H. Gao, L. Zhang

CELL **135.** Withdrawn.

CELL **136.** Aqueous dispersions of TEMPO-oxidized cellulose nanofi-brils with various metal counterions, and their super deodorant perfor-mances. **A. Sone**, T. Saito, A. Isogai

CELL **137.** Microwave-hydrothermal rapid synthesis of cellulose/Ag nano-composites and their antibacterial activity. **L. Fu**, Y. Liu, S. Liu, M. Ma

CELL **138.** Withdrawn.

CELL **139.** Sustainable polymer synthesized from gemini monomers. **Z. Wang**

CELL **140.** Analysis of Liquid Fuels from Thermal Depolymerization of Polypropylene in a Bench-Scale Reactor. **S.M. Cardinalli**, **J.M. Lemas**, S. Ramesh, J.E. Holm, C.J. Pope

CELL **141.** Conductive films prepared from cellulose, graphite and polyaniline nanoparticles with highly thermal stability and antibacterial activity. **J. Chen**, J. Liu, W. Zhang, K. Wang, X. Qian, R. Sun

CELL **142.** Recycling of non-metallic frac-tion of printed circuit boards as reinforce-ment in poly(methyl methacrylate) com-posites. **C. Loyo**, C. Arroyo, V. Valle, M. Aldas

CELL **143.** Applications of cellulosic waste. Development of insula-tion panels. L. Beltramini, R. Grether, **A. Guilarducci**, N. Ulibarrie

CELL **144.** Controlling latex morphol-ogy with cellulose nanocrystals and methyl cellulose. **S.A. Kedzior**, B. Morgan, E. Joy, Z. Hu, E.D. Cranston

CELL **145.** Synthesis of encapsulated bio-pesticides/fertilizers based on superabsorbent crosslinked alginate microbeads. **P. Joshi**, **M.L. Auad**

CELL **146.** Characterization of cellulose membrane filters deposited by electro-spinning. **J.L. Berrios-Rivera**, V. Pantojas

CELL **147.** Sequential fractionation of lignin macromolecules with organic solvents and investigation of their potentials for utilization as lignin-PLA copolymers. **S. Park**, J. Choi

CELL **148.** Development of reinforced rigid polyurethane foam composite based on cabuya fiber. **A. Proano**

CELL **149.** Biopolymer synthesis: Esterification of wood cellulose from different guatemalan tree species with phthalic anhydride and their use as triclosan adsorbents in aqueous solu-tions. **C.E. Torres**, J. Carrera, S. Toledo

CELL **150.** Cleavage of β-*O*-4 ether bonds in acidic lithium bromide trihydrate for lignin depolymeriza-tion. **N. Li**, X. Yang, X. Lin, X. Pan

CELL **151.** Conductive hydrogels for use in tissue engineering and biocompat-ible electronics. B. Cleary, **M.L. Auad**

CELL **152.** Preparation of electrospun mats of functionalized Nano-Crystalline Cellulose (NCC). R. Farag, Z. Jiang, B. Jackson, K. Brown, **M.L. Auad**

CELL **153.** Cellulose nanocrystal thin film swelling to probe parti-cle-particle interactions in solvents and aqueous media. **M.S. Reid**, S.A. Kedzior, M. Villalobos, E.D. Cranston

CELL **154.** Characterization of edible film based on zein and chi-tosan. **L. Pinho**, M. Oliveira, W.Q. Oliveira, R. Furtado, M.S. Bastos, F. R.W.

CELL **155.** Pre-treatments to create porous cellulose fibres for nanocellulose production. **M. Miranda**, C. Driemeier, A.J. Carvalho, N. Belgacem, **J. Bras**

CELL **156.** Succinylation of glucomannans from spruce for hydrogel formation. A. Escalante, K. Markstedt, P. Gatenholm, **G. Toriz Gonzalez**

CELL **157.** Biomass potential for the development of advanced materials and bio-based products. **M. Kurečič**, S. Hribernik, M. Bozic, A. Ojstršek, T. Kos, M. Mešl, K. Stana Kleinschek

CELL **158.** Gelation of 3D printed nanocellulose induced by crosslinked hemicellulose. **K. Markstedt**, A. Escalante, **G. Toriz Gonzalez**, P. Gatenholm

CELL **159.** Effect of the change of the crystalline structure on the infrared spectra by ATR of cellulose from banana rachis, corn husk and bacterial cellulose. **A.M. Serpa Guerra**, C. Gómez Hoyos, J.A. Velasquez- Cock, P. Gañán, C. Castro Herazo, R. Zuluaga Gallego

CELL **160.** Bacterial nanocellulose based bioink for 3D bioprinting. K. Markstedt, D. Hägg, T. Kondo, **G. Toriz Gonzalez**, P. Gatenholm

CELL **161.** Characterization of wood and cellulose from different eucalytpus species. **R. Teixeira Mendonça**, I. Carrillo, M. Pereira

CELL **162.** Biomaterial polymer blends for material extrusion 3D printing. **P. Tayeb**, L. Pal, A.H. Tayeb

CELL **163.** Solution/aggregation behavior of spruce xylan as function of isolation/purification conditions. **S. Kishani**, A. Escalante, **G. Toriz Gonzalez**, L. Wagberg, P. Gatenholm

CELL **164.** Extraction and characterization of nanocellulose from different biomass sources. **M. Alwohaibi**, C.J. Huntley, M.L. Curry

CELL **165.** Synthesis and fabrication of CNF-based plastic nanocomposites. **D.H. White**, C.J. Huntley, M.L. Curry

CELL **166.** Molecular blending and reinforcing effect of lignin in ductile epoxy resins. F. Ansari, **R. Rojas Escontrillas**, L. Berglund

CELL **167.** TEMPO- oxidized Nanofibrillated Cellulose Film (NFC) incorporating Graphene oxide (GO) nanofillers. **Y. Kim**, Y. Kim

CELL **168.** Enhanced solar driven water evaporation rates through graphitic surface film suspensions. **R. Christoph**, A. Hernández, R. Muñoz, S. Ventura

MONDAY MORNING

Section A

Moscone Center
252/260

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Structure

Cosponsored by CARB

Financially supported by EPNOE, Eastman Chemical Company, VT Fralin Life Science Institute, VT College of Natural Resources and Environment, VT Department of Sustainable Biomaterials, Carbohydrate Polymers (Elsevier)

C. M. Buchanan, P. E. Fardim, *Organizers*

O. J. Rojas, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **169.** Repeating unit of cellulose is glucose, and why that matters. **A.D. French**

8:30 CELL **170.** Findings on the way of cellulose ether analysis. **P. Mischnick**, K. Voiges, S. Gangula

8:55 CELL **171.** Withdrawn.

9:20 CELL **172.** Rheo-optical and optical studies of cellulose derivatives. **P.R. Navard**, T. Budtova

9:45 Intermission.

10:00 CELL **173.** Insights in the control of glycosaminoglycan structure. **R.J. Linhardt**

10:25 CELL **174.** Precision biomaterials based on synthetic heparan sulfate oligosaccharides. **G. Boons**

10:50 CELL **175.** New views of plant cell wall non-cellulosic polysaccharide and proteoglycan structure from studies of pectin biosynthetic enzymes and plants modified in their expression. **D. Mohnen**, M. Atmodjo, A. Biswal, R. Amos, K. Engle, L. Tan

11:15 CELL **176.** Conversion of agricultural by-products to methyl cellulose. **A. Biswas**, H. Cheng, R. Furtado, C.R. Alves

Section B

Moscone Center
262

Processing & Properties of Biobased Composites & Blends

Financially supported by EPNOE

P. R. Navard, *Organizer*

J. R. Barone, *Organizer, Presiding*

8:05 CELL **177.** Mechanical properties improvement of natural rubber/pineapple leaf fiber composites: Effects of silane treatment of fiber and incorporation of carbon black. **N. Hariwongsanupab**, K. Mougin, T. Amornsakchai, M. Vallat, S. Thanawan, G. Schrodj

8:30 CELL **178.** Substitution of formaldehyde in phenolic thermosets with innovative and bio-based lignin-to-vanillin derived compounds. **S. Caillol**

8:55 CELL **179.** Manufacturing strong regenerated cellulose fibers reinforced with cellulose nanocrystals. **J. Bhardwaj**, R. Richardson, J. Li, S. Rahatekar

9:20 CELL **180.** Micro and nano composites using cotton materials loaded in polylactic acid and applications in 3D printing. A. Kearns, **R.A. Venditti**, J. Jur, N. Farahbakhsh

9:45 Intermission.

10:00 CELL **181.** Design, fabrication and test of degradable starch based tube for a biomedical application. L. Chaunier, D. Velasquez, S. Guessasma, A. Bizeau, F. Faure, A. Meddahi-Pelle, **D. Lourdin**

10:25 CELL **182.** Blend configuration in polymeric materials with very high lignin-derivative contents. **S. Sarkanen**, Y. Wang, Y. Chen

10:50 CELL **183.** Lignin acidolysis predicts formaldehyde generation in pine wood. **C.E. Frazier**, G. Wan

11:15 CELL **184.** Amyloid reinforced polyvinyl alcohol nanocomposites. B.L. DeButts, **J.R. Barone**

Section C

Moscone Center
270

Cellulose Structure & Biosynthesis

Mechanism of Synthesis

Cosponsored by BIOL, BIOT, CARB and ENFL

Financially supported by Department of Energy - Office of Science

N. Carpita, D. Cosgrove, P. Langan, H. M. ONeill, *Organizers*

J. Zimmer, *Organizer, Presiding*

A. W. Roberts, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **185.** Structure and function of cellulose synthase. **J. Zimmer**

8:30 CELL **186.** Cellulose microfibril formation in vitro by a single heterologously expressed plant cellulose synthase isoform. **P. Pallinti**, S. Cho, S. Díaz-Moreno, M. Kumar, B. Nixon, V. Bulone, J. Zimmer

8:55 CELL **187.** All-atom structural models of plant cellulose synthase and cellulose synthase complex. A. Singh, S. Deshmukh, **Y.G. Yingling**

9:20 CELL **188.** Organization of domains in CESA proteins of the plant cellulose synthesis complex. **H.M. O'Neill**, V. Vandavasi, J. Du, Q. Zhang, A. Singh, B. Nixon, Y.G. Yingling, L. Petridis, P. Langan, C.H. Haigler

9:45 Intermission.

10:00 CELL **189.** Progress toward structural understanding of cellulose synthesis by plants. **B. Nixon**, M. Kumar, J. Du, S. Cho, V. Vandavasi, H.M. ONeill, P. Purushotham, J. Zimmer

10:25 CELL **190.** Cellulose structure and biosynthesis in oomycetes: Similitudes and differences with higher plants. **V. Bulone**

10:50 CELL **191.** Protein structural controls of plant cellulose synthesis. **C.H. Haigler**

11:15 CELL **192.** Structure of the catalytic domain of a plant CesA. P.S. Rushton, C. Rayon, A.T. Olek, L. Makowski, H. Kim, J. Badger, D. Kihara, C. Steussy, C.V. Stauffacher, **N. Carpita**

Section D

Moscone Center
272

Nanocellulose Processing & Analysis

Properties

Cosponsored by AGFD, ANYL, CHAS and I&EC

Financially supported by TAPPI

M. Bortner, W. Y. Hamad, T. Lindström, *Organizers*

M. Roman, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **193.** Solid-State and structural characterization of cellulose nanocrystals. **W.Y. Hamad**

8:30 CELL **194.** Comparing crystallinities of CNCs by Raman, NMR, and XRD. **U.P. Agarwal**, T. Larsson, J. Stevanic Srndovi

8:55 CELL **195.** Analysis of modified cellulose nanocrystals. **W. Thielemans**

9:20 CELL **196.** Characterization of nanocelluloses using small-angle neutron, x-ray and dynamic light scattering techniques. Y. Mao, K. Liu, C. Zhan, L. Geng, B.T. Chu, **B.S. Hsiao**

9:45 Intermission.

10:00 CELL **197.** Occupational health and safety characterization and assessment of CNC's from North American producers. **B. O'Connor**

10:25 CELL **198.** European perspective on Environmental, Health and Safety (EHS) aspects on Cellulose Nanofibrils (CNF). **H. Kangas**, M. Pitkänen, J. Catalan, H. Norppa

10:50 CELL **199.** TEMPO-Oxidized Cellulose Nanofiber (TOCN) materials show good biomedical applications. **N. Ruizhi**, L. Yi, S. Yamasaki, J. Lin, T. Saito, A. Isogai

11:15 CELL **200.** Different size-unified cellulose nanocrystals obtained via a multistage separation. **Y. Hu**, N. Abidi

11:40 Concluding Remarks.

Section E

Moscone Center
274

Functional Lignocellulosics & Nanotechnology

Tuning Interfacial Phenomena with Ligno-Nanocellulosic Materials

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, E. Filpponen, T. Nypelo, S. Peresin, S. Spirk, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **201.** Nanocellulose- Silver hybrid structuration for stable suspension and transparent conductive material design. **J. Bras**, F. Hoeng, A. Denneulin

8:30 CELL **202.** Control of the surface properties of cellulose nanocrystals by acylation with functional vinyl esters: Application to the design of innovative fillers or Pickering surfactants. **G. Sebe**, J. Brand, B. Dhuiege, A. Werner, V. Héroguez

8:55 CELL **203.** Click-Thiols as an approach to implement novel functionalities within bio-derived scaffolds. **S. Kostic**, J.K. Berg, K. Casdorff, V. Merk, I. Burgert, E. Cabane

‡ *Cooperative Cosponsorship*

9:20 CELL **204.** Cellulose nanocrystals and surfactants as mini emulsion polymerization stabilizers. **S.A. Kedzior**, H.S. Marway, E.D. Cranston

9:45 Intermission.

10:00 CELL **205.** Fundamental differences due to deposition method in ultrathin films of cellulose nanofibres. **B.P. Wilson**, K. Yliniemi, M. Gestranius, M. Putkonen, M. Lundström, T. Tammelin, E. Kontturi

10:25 CELL **206.** Tailor-made 3D printed scaffolds from cellulose nanofibrils for guided growth and development of a neural tissue. **V. Kuzmenko**, E. Karabulut, E. Pernevik, D. Hägg, S. Johannesson, P. Enoksson, P. Gatenholm

10:50 CELL **207.** 3D-printing of cellulosic materials – properties and suitability on cellulosic fabrics. **T. Tenhunen**, P. Varis, A. Puolakka, P. Kääriäinen, A. Harlin, M.K. Österberg, T. Tammelin, H. Orelma

11:15 CELL **208.** Cellulose macro-sheets with PTFE nanocoating and cellulose nano-sheets. **Y. Huang**, M. Wu, M. Zhao, S. Kuga

Section F

Moscone Center
276

Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy

Cosponsored by ENFL and ENVR

H. Mayes, C. J. Pope, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **209.** Hydrothermal carbonization and the circular economy. **M.T. Timko**

8:30 CELL **210.** Utilisation of microwave irradiation in the catalytic upgrade of cellulose and hemicellulose derivatives: Hydrolysis and hydrogenation reactions. **J. Lopez-Sanchez**

8:55 CELL **211.** Biomass vapor upgrading to produce hydrocarbon fuels. **C. Mukarakate**, K. lisa, M. Xu, M.R. Nimlos, J. Schaidle

9:20 CELL **212.** Oceans of plastic converted to liquid fuels via small scale thermal depolymerization reactors. **S. Ramesh**, **J.E. Holm**, C.J. Pope

9:45 Intermission.

10:00 CELL **213.** Data science tools for biomass pyrolysis – application to thermochemical conversion of lignin. **J. Pfaendtner**

10:25 CELL **214.** Mechanistic modeling of fast pyrolysis of hemicellulose extracted from cornstover. **X. Zhou**, W. Li, R. Mabon, L.J. Broadbelt

10:50 CELL **215.** On the importance of inorganics composition on biomass gasification. **D. Da Silva Perez**, C. Dupont

11:15 CELL **216.** Computational studies of lignin chemistry and structure. G. Beckham, L. Berstis, **M.F. Crowley**, R.A. Dixon, T.J. Elder, S. Kim, J. Vermaas

11:40 Concluding Remarks.

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

MONDAY AFTERNOON

Section A

Moscone Center
252/260

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Structure

Cosponsored by CARB

Financially supported by EPNOE, Eastman Chemical Company, VT Fralin Life Science Institute, VT College of Natural Resources and Environment, VT Department of Sustainable Biomaterials, Carbohydrate Polymers (Elsevier)

C. M. Buchanan, O. J. Rojas, *Organizers*

P. E. Fardim, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **217.** Chemistry with activated polysaccharide derivatives – an efficient and simple path to novel structures. **T.J. Heinze**, T. Elschner, M. Gericke, K. Ganske, F. Obst, L. Gabriel

1:30 CELL **218.** Withdrawn.

1:55 CELL **219.** LB film preparation of regioselectively substituted cellulose cinnamates on nematic ordered cellulose templates. **T. Kondo**

2:20 CELL **220.** Take advantage of what Nature creates and utilize biomass. **A. Albertsson**

2:45 Intermission.

3:00 CELL **221.** Enzymatic control of the acetylation pattern in chitosans. **B.M. Moerschbacher**

3:25 CELL **222.** Studying the reactivity of cellulose by oxidation with 4-acetamido-2,2,6,6-tetramethylpiperidine-1-oxo-piperidinium cation. **P. Khanjani**, V. Lovikka, T.C. Maloney, T. Vuorinen

Section B

Moscone Center
262

Processing & Properties of Biobased Composites & Blends

Financially supported by EPNOE

P. R. Navard, *Organizer*

J. R. Barone, *Organizer, Presiding*

J. Ganster, *Presiding*

1:05 CELL **223.** Orientation and interfacial stress transfer of cellulose nanocrystal nanocomposite fibers. **H. Chang**, J. Luo, H.C. Liu, A. Bakhtiary Davijani, P. Wang, S. Kumar

1:30 CELL **224.** Understanding nanoconfinement and nanoscale interfaces in nanocellulose composites. **S. Keten**

1:55 CELL **225.** Enhancing supramolecular interactions in aromatic polymer/cellulose nanocrystals nanocomposites. E. Rivoire, A. Garcia, A. Saralegi, J. Foster, **J. Bras**

2:20 CELL **226.** Excellent dispersion and property enhancements in polymer composites made with biobased filler from cellulose nanocrytals and waste paper to lignin and agro-waste to rice husk ash and eggshell. **J.M. Torkelson**, K.A. Iyer, G.T. Schueneman

2:45 Intermission.

3:00 CELL **227.** Amyloid reinforced rubber nanocomposites. B.L. DeButts, L.E. Hanzly, **J.R. Barone**

3:25 CELL **228.** Melt mixing cellulose nanocrystals and industrially relevant polymers. **J. Foster**

Section C

Moscone Center
270

Cellulose Structure & Biosynthesis

Synthase Trafficking & Synthesis of plant (1->3),(1->4)-D-glucans

Cosponsored by BIOL, BIOT, CARB and ENFL

Financially supported by Department of Energy - Office of Science

N. Carpita, D. Cosgrove, P. Langan, J. Zimmer, *Organizers*

H. M. ONeill, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **229.** Cellular mechanisms of CESA trafficking and delivery to the plasma membrane. T. Vellosillo, R.X. Gutierrez, C.R. Somerville, **D.W. Ehrhardt**

1:30 CELL **230.** Does cortical microtubule array guide the orientation of cellulose deposition or not? **Y. Gu**

1:55 CELL **231.** Myosins XI are involved in cellulose synthase complex dynamics and delivery. W. Zhang, C. Cai, N. Carpita, **C.J. Staiger**

2:20 CELL **232.** Real-time imaging of cellulose microfibril and biosynthesis. **S. Ding**

2:45 Intermission.

3:00 CELL **233.** Understanding the mechanism of (1,3;1,4)-β-D-glucan synthesis in cereals. **M. Doblin**, Y. Ho, D. Oehme, M.P. Bain, K. Ford, A.M. van de Meene, E.R. Lampugnani, A. Bacic

3:25 CELL **234.** Characterizing and utilizing CSLF6 to improve MLG synthesis. **S. Kim**, S. Zemelis-Durfee, K. Keegstra, F. Brandizzi

Section D

Moscone Center
272

Nanocellulose Processing & Analysis

Fundamentals

Cosponsored by AGFD, ANYL, CHAS and I&EC

Financially supported by TAPPI

M. Bortner, T. Lindström, M. Roman, *Organizers*

W. Y. Hamad, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **235.** Cellulose bio-inspired hierarchical structures. **S. Vignolini**, R. Parker, B. Frka-Petesic, G. Guidetti

1:30 CELL **236.** Driving forces for cellulose nanocrystal alignment in drying droplets: Center versus edge. F. Navarro Arzate, **C. Pritchard**, M. Bortner, **M. Roman**

1:55 CELL **237.** *In-situ* small angle X-ray scattering of a levitated cellulose nanocrystal droplet. **Y. Liu**, M. Agthe, A. Fall, G. Salazar-Alvarez, C. Schütz, L. Bergstrom

2:20 CELL **238.** *In situ* Rheo-SAXS study of cellulose nanocrystals suspensions. A. De Geyer, C. Rey, N. Hengl, E. Gicquel, J. Bras, **B.R. Jean**, F. Pignon

2:45 Intermission.

3:00 CELL **239.** Effect of the size of the charged group on the properties of alkoxylated NFCs. **A. Naderi**, T. Larsson, J. Stevanic Srndovi, T. Lindström, J. Erlandsson

3:25 CELL **240.** Interaction of β-(1-4) xylan with cellulose surface in biomimetic reconstructed models. L. Falcoz-Vigne, Y. Ogawa, V. Meyer, M. Petit-Conil, K. Mazeau, Y. Nishiyama, **L. Heux**

3:50 Concluding Remarks.

Section E

Moscone Center
274

Functional Lignocellulosics & Nanotechnology

Modification & Analytics

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, T. Nypelo, S. Peresin, S. Spirk, *Organizers*

E. Filpponen, *Organizer, Presiding*

R. Kargl, *Presiding*

1:05 CELL **241.** Periodate oxidation and chemical modifications of cellulosic backbone. **J. Leguy**, Y. Nishiyama, L. Heux, B.R. Jean

1:30 CELL **242.** Designer molecules for one-step modification of cellulosic materials in aqueous and organic media through the triazine chemistry. **A. Fatona**, R.M. Berry, M.A. Brook, J. Moran-Mirabal

1:55 CELL **243.** Dissolution of cellulose in NaOH/zinc nitrate at low temperature. **A. Lyu**

2:20 CELL **244.** Withdrawn.

2:45 Intermission.

3:00 CELL **245.** Topochemical modification of nanocellulose in ionic liquids or gamma-valerolactone. T. Laaksonen, **A. King**, J.K. Helminen, L. Lemetti, D. Rico del Cerro, I. Filpponen, M. Kemell, S. Heikkinen, I. Kilpeläinen

3:25 CELL **246.** Essential analytical approaches to characterization of lignin specifically targeting the abundant oligomeric fraction observed following a hydrotreatment. **A. Kubatova**, A. Andrianova, J. Kreft, K. Voeller, J. Schumaker, E.I. Kozliak, I.P. Smoliakova

Section F

Moscone Center
276

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

M. L. Auad, J. Campos-Teran, *Organizers*

O. J. Rojas, *Organizer, Presiding*

M. Ago, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **247.** Silylated lignin and copolymers with acrylonitrile: Flexible membranes and material precursors. **S. Li**, W. Xie, M. Wilt, J.A. Willoughby, O.J. Rojas

1:30 CELL **248.** Grafting-from cellulose via photoinduced Cu-mediated reversible deactivation radical polymerisation. **F. Hatton**, S.A. Kedzior, E. Larsson, E.D. Cranston, A.E. Carlmark

1:55 CELL **249.** Valorization of lignin in 0D and 1D advanced systems: Particles for emulsification and fibers for energy storage. **M. Ago**, T. Kämäräinen, B. Tardy, S. Huan, M. Borghei, J. S. Haataja, J. Raula, E.I. Kauppinen, O.J. Rojas

2:20 CELL **250.** Synthesis, properties and carbonization of different types of ligneous aerogels. **E. Budjav**, S. Quraishi, M. Ghorbani, J. Konnerth, C. Unterweger, F. Liebner

2:45 Intermission.

3:00 CELL **251.** Fiber-based foams for papermaking. **W. Xiang**, I. Filpponen, E. Saharinen, K. Salminen, T. Lappalainen, O.J. Rojas

3:25 CELL **252.** Towards a better understanding of alkali-lignins isolated from three kinds of non-woody materials. **F. Yue**, F. Lu, R. Sun, J. Ralph

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Carbohydrate-Based Hybrid Materials for Nanomedicine

Sponsored by CARB, Cosponsored by CELL

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

M. Roman, *Organizer*

8:00 - 10:00

40, 43-45, 60, 97, 98-101, 106, 108-110, 112, 114-116, 118, 121, 124-125, 129, 134-135, 137-140, 142, 146, 148-149, 154, 159, 162, 164-165, 167, 177, 203, 206, 215, 233, 242, 244, 251. See previous listings.

262-263, 299, 347, 351, 528. See subsequent listings.

TUESDAY MORNING

Section A

Moscone Center

252/260

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Novel Derivatives for Demanding Applications

Cosponsored by CARB

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Financially supported by EPNOE, Eastman Chemical Company, VT Fralin Life Science Institute, VT College of Natural Resources and Environment, VT Department of Sustainable Biomaterials, Carbohydrate Polymers (Elsevier)

C. M. Buchanan, P. E. Fardim, *Organizers*

O. J. Rojas, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **253.** Control of optical anisotropy of cellulose derivatives. **M. Yamaguchi**, H. Shimada, K. Songsurang

8:30 CELL **254.** Design of optical films for liquid crystalline displays by control of cellulose ester structure. **C.M. Buchanan**, N. Buchanan, E. Guzman-Morales, B. Wang

8:55 CELL **255.** Nano- and micropatterns of cellulose - from lithography to microphase separation. K. Niegelhell, H. Plank, F. Stelzer, R. Kargl, T. Griesser, **S. Spirk**

9:20 CELL **256.** Photo- and biodegradable thermoplastic elastomers containing cellulose and polylactide. **J.B. Matson**, K.J. Arrington

9:45 Intermission.

10:00 CELL **257.** Heterogeneous catalysts for the regioselective modification of cellulose. **S. Renneckar**, S.C. Patankar

10:25 CELL **258.** Control of cellulose chiral nematic structure. **D.G. Gray**

10:50 CELL **259.** Looking at the unwanted acetylation of polysaccharides by 1,3-dialkylimidazolium acetate ionic liquids: Analysis, acetylating agent, influence of water, and mechanistic considerations. **T. Rosenau**, A. Potthast, M. Laborie, T. Zweckmair, H. Hettegger, M. Bacher, H. Abushammala

11:15 CELL **260.** Peptide-cellulose conjugates for protease point of care diagnostics and treatment. **V. Edwards**, K.R. Fontenot, N.T. Prevost, F. Liebner, A.D. French, D. Haldane, N. Pircher, B.D. Condon

Section B

Moscone Center

262

Processing & Properties of Biobased Composites & Blends

Financially supported by EPNOE

P. R. Navard, *Organizer*

J. R. Barone, *Organizer, Presiding*

L. Averous, *Presiding*

8:05 CELL **261.** New biobased and sustainable epoxy and polyurethane materials and foams from vegetable and microalgal oil. **S. Caillol**

8:30 CELL **262.** Polylactide/ZnO nanocomposites: From improved functional properties for packaging to novel materials for biomedicine. **E. Lizundia**, J.L. Vilas

8:55 CELL **263.** Green composites from hemp fibers and styrene-free soybean oil-based thermosets: Preparation and modification. W. Liu, **R. Qiu**

9:20 CELL **264.** Thermal superinsulating silica aerogels and xerogels reinforced with short cellulose fibers. G. Markevicius, J. Jaxel, P. Niemeyer, R. Ladj, A. Rigacci, **T. Budtova**

9:45 Intermission.

10:00 CELL **265.** Biopolymer-based multilayer nanocoatings that exhibit high gas barrier and flame retardant behavior. **J.C. Grunlan**

10:25 CELL **266.** Withdrawn.

10:50 CELL **267.** Comparative studies on miscibility and intermolecular interaction for cellulose ester blends with vinyl copolymers. **K. Sugimura**, Y. Nishio

11:15 CELL **268.** Sustainable polymeric materials via strategic assemblies of renewable platform chemicals. **J.M. Sadler**, J.F. Stanzione, G.R. Palmese, J.J. La Scala

Section C

Moscone Center

270

Cellulose Structure & Biosynthesis

Biochemistry & Cellular Biology

Cosponsored by BIOL, BIOT, CARB and ENFL

Financially supported by Department of Energy - Office of Science

D. Cosgrove, P. Langan, H. M. ONeill, J. Zimmer, *Organizers*

N. Carpita, *Organizer, Presiding*

M. Doblin, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **269.** Characterization of *Arabidopsis* CSLD cell wall synthase activities both *in vitro* and *in vivo*. G. Bak, F. Gu, J. Combs, M. Pena, B. Urbanowicz, **E. Nielsen**

8:30 CELL **270.** Golgi-localized STELLO proteins regulate the assembly and trafficking of cellulose synthase complexes. Y. Zhang, N. Nikolovksi, M. Sorieul, T. Vellosillo, H. McFarlane, R. Dupree, C. Driemeier, J. Mortimer, S.P. Brown, S. Persson, **P. Dupree**

8:55 CELL **271.** Sphingolipid glycosylation in plants: Some implications for cellulose biosynthesis. L. Fang, B. Jing, T. Ishikawa, E. Rennie, H.V. Scheller, **J.C. Mortimer**

9:20 CELL **272.** Functional differences between CESA protein classes. **S. Turner**, M. Kumar, L. Mishra

9:45 Intermission.

10:00 CELL **273.** Brassinosteroids regulate cellulose biosynthesis in *Arabidopsis thaliana* by direct phosphorylation. **I.S. Wallace**, K.J. Ketelaar, C. Sanchez-Rodriguez, R. Schneider, J.A. Villalobos, C.R. Somerville, S. Persson

10:25 CELL **274.** Ultrastructure of spruce secondary wall outer layers. **M. Reza**, C. Bertinetto, J. Ruokolainen, T. Vuorinen

10:50 CELL **275.** Investigating inter-fibrillar distance between crystalline cellulose microfibrils in plant cell walls using sum frequency generation vibrational spectroscopy. **A. Makarem**, D. Sawada, H.M. O'Neill, S.H. Kim

11:15 CELL **276.** Bacterial cellulose: Self-assembly and reformatting. **S. Lim**

Section D

Moscone Center

272

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Cosponsored by AGFD, ANYL and POLY

Financially supported by HORIBA Instruments Incorporated; University of Tokyo, Japan; Innventia AB; U.S. Forest Service

U. P. Agarwal, T. J. Elder, A. Isogai, T. Larsson, *Organizers*

A. D. French, T. Rosenau, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **277.** Evolving models of lignocellulose structure: Do we need a plant cell wall interactome. **W.T. Winter**

8:30 CELL **278.** Chain polarity in polymorphic unit cells of cellulose, amylose, and chitin. **S.H. Kim**

8:55 CELL **279.** Enzymatic oxidation of carbohydrates: New applications and new paradigms for lignocellulose deconstruction. **C. Felby**, K.B. Møllers, D. Cannella

9:20 CELL **280.** ^{13}C NMR method for characterization of partially dissolved cellulose in aqueous media. **D. Topgaard**

9:45 Intermission.

10:00 CELL **281.** Disordered structures in plant cellulose microfibrils in terms of leveling-off DP and layer-by-layer surface peeling of microfibrils. **A. Isogai**

10:25 CELL **282.** Multifunctional cellulose derivatives for surface modification – an innovative nanostructural approach. **T.J. Heinze**, P.E. Fardim

10:50 CELL **283.** Fire protection of cellulose materials, procedures and mechanisms. **L. Wagberg**, M. Ghanadpour, O. Koklukaya, F. Carosio

11:15 CELL **284.** Use of Raman microscopy in elucidating the structure of cellulose. **F. Adar**

Section E

Moscone Center

274

Functional Lignocellulosics & Nanotechnology

Tuning Interfacial Phenomena with Ligno-Nanocellulosic Materials

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, E. Filpponen, T. Nypelo, S. Peresin, S. Spirk, *Organizers*, *Presiding*

8:05 CELL **285.** Nanoscale self-assembling properties of hybrid materials obtained from hemicelluloses oligomers and fatty acids in polar and non-polar media. **D. Da Silva Perez**, M. Chemin, J. Russelgong, H. Cramail, S. Grelier

8:30 CELL **286.** Xyloglucan functional block-copolymers: A modular platform for cellulose modification. F. Hatton, J. Engström, J. Forsling, E.E. Malmstrom, M. Ruda, F. D'Agosto, M. Lansalot, **A.E. Carlmark**

8:55 CELL **287.** Spruce galactoglucomannans stabilize emulsions against physical breakdown and lipid oxidation. **K. Mikkonen**, M. Lehtonen, D. Merger, U. Van der Schaaf, P. Kilpeläinen, C. Xu, C. Berton, M. Wilhelm, K. Schroën

‡ *Cooperative Cosponsorship*

9:20 CELL **288.** Parametric analysis and mechanism of dispersion of single-walled and multi-walled carbon nanotubes by cellulose nanocrystals. J. Mougel, B. Patricia, I. Capron, **B. Cathala**, O. Chauvet

9:45 Intermission.

10:00 CELL **289.** Exclusive surface modification of cellulose nanopapers by adsorption of polymers from non-aqueous solvents. **K.S. Kontturi**, K. Biegaj, A. Mautner, R.T. Woodward, B.P. Wilson, K. Lee, J. Heng, A. Bismarck, E. Kontturi

10:25 CELL **290.** New insights on the effects of chemical structure on the properties of cellulose nanofibrils: Characterization, mechanical performance and barrier properties. **V. Lopez Duran**, P.A. Larsson, L. Wågberg

10:50 CELL **291.** Tannic acid – A transformative additive when combined with cellulose nanocrystals: From hydrophobic nanoparticles to dried oil powders. **E.D. Cranston**, Z. Hu, R.H. Pelton

11:15 CELL **292.** Cellulose nanoparticles stabilized in a hydrophobic polymer matrix through synthetic functionalization. B. Teipel, R. Vano, M. Kirby, B. Zahner, E. Teipel, **N. Nagabandi**, K. Holder, M. Akbulut

Section F

Moscone Center

276

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

M. L. Auad, J. Campos-Teran, *Organizers*

O. J. Rojas, *Organizer, Presiding*

G. Toriz Gonzalez, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **293.** Dissolution and processing of lignocellulose using an ionic liquid solvent: Towards the production of high performance materials. **M. Hummel**, S. Hellsten, S. Asaadi, Y. Ma, E. Walger, S. Haslinger, H. Sixta

8:30 CELL **294.** Enzymatically produced lignosulfonate based paper coatings for substitution of petroleum based additives. **A. Ortner**, K. Hofer, S. Kopacic, G. Nyanhongo, W. Bauer, G.M. Guebitz

8:55 CELL **295.** Surface wrinkling phenomena in spherical lignin nano- and micro-particles obtained by aerosol flow synthesis. **T. Kämäräinen**, M. Ago, B. Tardy, J. Seitsonen, O.J. Rojas

9:20 CELL **296.** Wood waste: Resource of biopolymers and high value materials. **L. Couret**, B. Cathala, E. Bonnin, C. Belloncle, M. Irle

9:45 Intermission.

10:00 CELL **297.** Valorization of lignin and cellulose in acid-steam-exploded corn stover by a moderate alkaline ethanol post-treatment based on an integrated biorefinery concept. S. Yang, **T. Yuan**, R. Sun

10:25 CELL **298.** Functional materials from spruce hemicelluloses: Crosslinkable xylans and glucomannans. **G. Toriz Gonzalez**, A. Escalante, P. Gatenholm, K. Markstedt

10:50 CELL **299.** Withdrawn.

LPS: Chemistry, Synthesis & Applications

Sponsored by CARB, Cosponsored by CELL

Carbohydrate-Based Hybrid Materials for Nanomedicine

Sponsored by CARB, Cosponsored by CELL

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

TUESDAY AFTERNOON

Section A

Moscone Center

252/260

Design & Control in Polysaccharide Chemistry: Anselme Payen Award Symposium in honor of Kevin J. Edgar

Novel Derivatives for Demanding Applications

Cosponsored by CARB

Financially supported by EPNOE, Eastman Chemical Company, VT Fralin Life Science Institute, VT College of Natural Resources and Environment, VT Department of Sustainable Biomaterials, Carbohydrate Polymers (Elsevier)

P. E. Fardim, O. J. Rojas, *Organizers*

C. M. Buchanan, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **300.** Olefin cross-metathesis: Mild, efficient and modular pathway to a new world of polysaccharide derivatives for drug delivery applications. **Y. Dong**, L.I. Mosquera-Giraldo, L. Taylor, K.J. Edgar

1:30 CELL **301.** Overview of TEMPO-mediated oxidation of polysaccharides. **A. Isogai**

1:55 CELL **302.** Synthesis, properties, and applications of cellulosic diblock copolymers. **H. Kamitakahara**

2:20 CELL **303.** Self-healing materials from cellulose. **G. Wenz**, D. Hafner

2:45 Intermission.

3:00 CELL **304.** Oxidative enzymes - route to functional polysaccharides. **M. Tenkanen**, A. Ghafar, I. Nikkilä, K. Parikka, K. Mikkonen

3:25 CELL **305.** Functionalized and sequence-defined polysaccharides by glycosynthase-catalyzed polymerization. **A. Planas**

3:50 CELL **306.** Design and control in polysaccharide chemistry. **K.J. Edgar**

Section B

Moscone Center

262

Processing & Properties of Biobased Composites & Blends

Financially supported by EPNOE

P. R. Navard, *Organizer*

J. R. Barone, *Organizer, Presiding*

J. Bras, *Presiding*

1:05 CELL **307.** Comparison of biobased multiphase systems based on different thermoplastic polysaccharides (starch, chitosan and alginate) obtained by thermomechanical mixing. **L. Averous**, E. Pollet

1:30 CELL **308.** Melt processing of functional protein/polymer blends. **J.K. Pokorski**, P. Lee

1:55 CELL **309.** Compression molded composites from waste polyester and cotton textiles. H. Xu, M. Palakurthi, L. Xu, **Y. Yang**

2:20 CELL **310.** Crucial role of processing regimes and compatibilization for toughening highly lignin filled polyethylene blends. **J. Ganster**, J. Erdmann

2:45 Intermission.

3:00 CELL **311.** Morphological and structural investigation of cellulose I and II nanocrystals. W. Flauzino Neto, J. Putaux, M. Mariano, Y. Ogawa, H. Otaguro, D. Pasquini, **A. Dufresne**

3:25 CELL **312.** Thin ply bacterial cellulose-reinforced polylactide nanocomposites. **M. Hervy**, F. Bock, K. Lee

Section C

Moscone Center

270

Advances in Polysaccharides: Practice & Applications

New Developments in the Industrial Sector

Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

A. Biswas, H. Cheng, *Organizers*

H. Cheng, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **313.** New family of cellulosic excipients for poorly-soluble actives. **R.L. Sammler**, T. Chatterjee, W. Porter, K. O'Donnell

1:30 CELL **314.** New understanding of syneresis in cellulose ether hydrogels. **C.E. Mohler**, R.L. Sammler, T. Sanders Jr, B. Huebner-Keese, J.D. Moore, T. Boomgaard

1:55 CELL **315.** Development of extrudable derivatives of Hypromellose Acetate Succinate (HPMC-AS) polymer excipient for use in drug solubilization enhancement. **T.A. Brugel**, F.J. Kolpak, S.K. Sahoo, Q. Schwing, D. Tewari

2:20 CELL **316.** Bacterially derived medical devices: How commercialization of cellulose requires redefining standard industrial practice. **W. Czaja**, **D. Inselman**, **E. Shwarz**

2:45 Intermission.

3:00 CELL **317.** Development of cellulose-based bioplastic featuring high optical characteristics of traditional Japanese lacquerware: Urushi black bioplastic. **K. Toyama**, M. Iji, Y. Shimode, H. Hamada

3:25 CELL **318.** New approaches to measure domain sizes in multi-component cellulosic derivatives using NMR. **S. Schantz**, J. Schlagnitweit, M. Tang, M. Baias, A.J. Rossini, S. Richardson, L. Emsley

Section D

Moscone Center

272

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Cosponsored by AGFD, ANYL and POLY

Financially supported by HORIBA Instruments Incorporated; University of Tokyo, Japan; Innventia AB; U.S. Forest Service

U. P. Agarwal, A. Isogai, T. Larsson, *Organizers*

T. J. Elder, *Organizer, Presiding*

W. T. Winter, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **319.** Monitoring structural changes during fibrillation of cellulose pulp into cellulose nanofibrils. J. Mao, B. Heck, H. Abushammala, G. Reiter, **M.G. Laborie**

1:30 CELL **320.** Use of *in vitro* biosynthetic systems to understand cellulose formation and properties. **V. Bulone**

1:55 CELL **321.** Structure-property relationships of nanocellulose fibrils. **G. Nyström**

2:20 CELL **322.** Withdrawn.

2:45 Intermission.

3:00 CELL **323.** Changes in the supra-molecular structure of cellulose I during TEMPO-oxidation. Bringing together NMR, MD, and XRD results. **T. Larsson**, J. Wohlert, M. Bergenstråhle

3:25 CELL **324.** Mechanical performance of CNF films revealed by Raman spectroscopy. **S.J. Eichhorn**, T. Tammelin, N. Wanasekara, A. Lewandowska, V. Kunnari, T. Kalijunen

Section E

Moscone Center

274

Functional Lignocellulosics & Nanotechnology

Dispersions, Gels, Foams, Colloids & Films

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, E. Filpponen, S. Peresin, S. Spirk, *Organizers*

T. Nypelo, *Organizer,Presiding*

A. King, *Presiding*

1:05 CELL **325.** Structural evaluation of cellulose-coated oil-in-water emulsions formed from solution. **Y. Cohen**, S. Napso, G. Alfassi, H. Miyamoto, D. Rein, R. Khalfin

1:30 CELL **326.** Organisation of cellulose ester monolayers on solid substrates upon Langmuir-Schaefer deposition. **E. Niinivaara**, B.P. Wilson, A. King, E. Kontturi

1:55 CELL **327.** Photo-induced thiol-ene functionalization towards superhydrophobic and slippery lubricant-infused nanocellulose films. **J. Guo**, W. Fang, A. Welle, W. Feng, E. Filpponen, O.J. Rojas, P. Levkin

2:20 CELL **328.** Effect of cellulose nanocrystal chirality on the stereochemistry of surface-tethered polymers. **J.O. Zoppe**, A.V. Dupire, H.A. Klok

2:45 Intermission.

3:00 CELL **329.** Tailoring the surface wettability of cellulose paper/nanopaper via photo-induced click reactions. J. Guo, L. Johansson, **E. Filpponen**, P. Levkin, O.J. Rojas

3:25 CELL **330.** Nanocellulose as rheology modifier of drilling fluids – Thermostability of nanocellulose dispersions. **K. Syverud**, E. Heggset, G. Chinga-Carrasco

Section F

Moscone Center

276

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

M. L. Auad, J. Campos-Teran, *Organizers*

O. J. Rojas, *Organizer, Presiding*

C. G. Hunt, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **331.** Potential use of pulp and paper industry side streams in composites. **L. Wikström**, J. Keränen

1:30 CELL **332.** Experimental test of limited oxidant diffusion mechanism of decay resistance in acetylated wood. **C.G. Hunt**, S. Lacher, K. Hirth, L. Lorenz, E. Engelund Thybring, S.L. Zelinka

1:55 CELL **333.** Biocatalytic films based on lignin, cationic polymers and immobilized lipase layers. **M.H. Sipponen**, T. Leskinen, J. Valle-Delgado, M.K. Österberg

2:20 CELL **334.** Identification of accumulated carbohydrate degradation products during the processing of cellulose using an ionic liquid solvent: Towards solvent recycling. **E. Walger**, S. Hellsten, J. Witos, S. Wiedmer, M. Hummel, H. Sixta

2:45 Intermission.

3:00 CELL **335.** Industrial biorefinery of lignocellulose for production of biomaterials in China. **R. Sun**

3:25 CELL **336.** Wood component separation by dilute acid prehydrolysis with *p*-cresol. **H. Tomoyuki**, H. Nonaka

LPS: Chemistry, Synthesis & Applications

Sponsored by CARB, Cosponsored by CELL

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

WEDNESDAY MORNING

Section A

Moscone Center

252/260

Bio-based Gels & Porous Materials

Biopolymer Hydrogels

Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Financially supported by EPNOE

T. Budtova, F. Liebner, *Organizers*

N. Abidi, R. Sun, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **337.** Insight into mild condition dissolution of high molecular weight cellulose in ionic liquid based solvent system. S. Acharya, Y. Hu, **N. Abidi**

8:30 CELL **338.** Soft gelation of cellulose/DMAc/LiCl solution. **R. Liu**, C. Zhang, J. Xiang, H. Kang, Y. Huang

8:55 CELL **339.** Cellulose gels and cryogels via physical and chemical cross-linking. D. Ciolacu, C. Rudaz, M. Vasilescu, **T. Budtova**

9:20 CELL **340.** New cellulosic sponge and foam made from cellulose fibers through a simple freezing/thawing method. **A. Tejado**, A. Aramburu, Y. de Miguel

9:45 Intermission.

10:00 CELL **341.** Rheological behavior of thermosensitive hydrogel suspensions based on Cellulose Nanocrystals with adsorbed thermo-responsive polymer. **E. Gicquel**, B. Jean, J. Engström, C. Martin, A.E. Carlmark, J. Bras

10:25 CELL **342.** Nanocellulose based electrospun membranes for water purification: Tailoring of porosity and functionality. **A. Mathew**

10:50 CELL **343.** Robust, dynamic hydrogels with modified cellulose nanocrystals as crosslinkers. **K. Zhang**

11:15 CELL **344.** Lignin-based hydrogels with super-swelling capacities. **J. Domínguez-Robles**, A. Jaaskelainen, A. Rodríguez, T. Tamminen, T. Liitiä, E. Larrañeta, M.S. Peresin

Section B

Moscone Center

262

Processing & Properties of Biobased Composites & Blends

Financially supported by EPNOE

J. R. Barone, P. R. Navard, *Organizers*, *Presiding*

8:05 CELL **345.** Potential of cellulosic nanocomposites materials from cassava pulp. **K. Kasemwong**, K. Piyachomkwan

8:30 CELL **346.** Various shapes of chitosan based nanocomposites and their hemostatic ability. **Y. Bao**, S. Wu, X. Shi, H. Deng, **Y. Du**

8:55 CELL **347.** Degradation kinetics of compression-molded date pits composites. **A. Mohamed**, S. Hussain, M. Alamri

9:20 CELL **348.** Fiber, a wonderfull from plantain crop residues. Alternative for human sustainable development. **O.E. Suarez Moreno**, M. Correa Velez

9:45 Intermission.

10:00 CELL **349.** Cotton-based cellulose nanomaterials for applications in composites and electronics. N. Farahbakhsh, **R.A. Venditti**, J. Jur

10:25 CELL **350.** Interfacial thickness for tailoring the reinforcing properties of nanocellulose in polymer matrix. **H. Soeta**, T. Saito, A. Isogai

10:50 CELL **351.** Transparent, macro to nano moldable composites reinforced by cellulose nanofibers. **S.K. Biswas**, H. Yano

11:15 CELL **352.** Functional cellulose nanocrystal reinforcing fillers in polymer nanocomposite films. **J.A. Sirviö**, M. Visanko, J.P. Heiskanen, H. Liimatainen

Section C

Moscone Center

270

Advances in Polysaccharides: Practice & Applications

Novel Biocatalytic & Biopolymeric Approaches

Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

A. Biswas, H. Cheng, *Organizers*

G. W. Selling, *Presiding*

8:05 CELL **353.** Chemo-enzymatic synthesis and functional properties of well-defined human milk oligosaccharides. **G. Boons**

8:30 CELL **354.** Chemo-enzymatic synthesis of homogeneous hyaluronan polysaccharides and their biological applications. J. Fang, **P.G. Wang**

8:55 CELL **355.** Chemoenzymatic synthesis of carbohydrates and glycoconjugates. **X. Chen**

9:20 CELL **356.** Structure and property of new dextrans obtained by enzymatic synthesis. **P. Faucard**, F. Grimaud, A. Rolland-Sabaté, M. Remaud-Siméon, G. Potocki-Véronèse, D. Lourdin

9:45 Intermission.

10:00 CELL **357.** Enzymatic production of oligosaccharides and polysaccharides for food ingredient applications. **R. DiCosimo**

10:25 CELL **358.** Synthesis of well-defined unnatural polysaccharides by phosphorylase-catalyzed enzymatic polymerization. **J. Kadokawa**

10:50 CELL **359.** Combined enzymatic-ionic liquid treatments to increase the accessibility and reactivity of pulp fibers. **R. Wahlström**, J. Rahikainen, K. Kruus, A. Suurnäkki

11:15 CELL **360.** Dendrimer-like biopolymers: A new arena for biomaterial development. **Y. Yao**

Section D

Moscone Center

272

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Cosponsored by AGFD, ANYL and POLY

Financially supported by HORIBA Instruments Incorporated; University of Tokyo, Japan; U.S. Forest Service

T. J. Elder, A. Isogai, T. Larsson, *Organizers*

U. P. Agarwal, *Organizer, Presiding*

O. J. Rojas, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **361.** Cellulose crystallinity: What does it mean? **M.F. Crowley**, M. Himmel, L. Bu, Y. Zhang, L. Makowski

8:30 CELL **362.** Visualization of dynamic changing in formation of cell wall cellulose and callose along with arrangements of microtubules with GFP on surfaces of protoplast cells. **T. Kondo**, S. Tagawa

8:55 CELL **363.** Explicit modeling and underdetermined (scattering) data to approach a complex reality. **Y. Nishiyama**

9:20 CELL **364.** Folding of xylan onto cellulose fibrils in plant cell walls revealed by solid-state NMR. T.J. Simmons, J. Mortimer, O.D. Bernardinelli, A. Poppler, S.P. Brown, E. Azevedo, R. Dupree, **P. Dupree**

9:45 Intermission.

10:00 CELL **365.** Cellulose II formation by cellulose synthase: Negative data can make themselves positive? **T. Imai**, J. Sugiyama

10:25 CELL **366.** Towards an improved understanding of cellulose swelling, dissolution and regeneration at the molecular level. **T. Rosenau**, A. Potthast

10:50 CELL **367.** Evolution of our understanding of native celluloses. **R.H. Atalla**

Section E

Moscone Center

274

Functional Lignocellulosics & Nanotechnology

Dispersions, Gels, Foams, Colloids & Films

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, E. Filpponen, T. Nypelo, S. Spirk, *Organizers*

S. Peresin, Organize,*Presiding*

T. J. Elder, *Presiding*

8:05 CELL **368.** Hydrolysis assisted by hydrogen chloride vapor on different cellulose polymorphs. **E. Kontturi**, E. Niinivaara, S.A. Arshath, A. Bismarck

8:30 CELL **369.** Crosslinking as a facilitator for novel (nano)cellulose-based applications. **P.A. Larsson**, J. Erlandsson, V. Lopez Duran, J. Henschen, N. Tchang Cervin, Z. Al-Ansari, A.J. Svagan, L. Wagberg

8:55 CELL **370.** Withdrawn.

9:20 CELL **371.** Oriented all-cellulose film based on ramie fiber with high mechanical property and transparency. **X. Yang**, L. Berglund

9:45 Intermission.

10:00 CELL **372.** Sample geometry dependency on the measured tensile properties of cellulose nanopapers. M. Hervy, A. Santmarti, P. Lahtinen, T. Tammelin, **K. Lee**

10:25 CELL **373.** Enzymatic and chemical modifcation of nanosized colloidal lignin particles. J. Valle-Delgado, T. Leskinen, A. Paananen, M.K. Österberg, **M. Mattinen**

10:50 CELL **374.** Partial dissolution as a reinforcing chemistry for CNF films. **H. Orelma**, A. Korpela, V. Kunnari, A. Harlin, T. Tammelin, A. Suurnäkki

11:15 CELL **375.** Water-resistant nanocellulose films with inter-fibrillar interactions via multivalent metal ions. **M. Shimizu**, T. Saito, A. Isogai

‡ *Cooperative Cosponsorship*

Section F

Moscone Center
276

Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

J. Campos-Teran, O. J. Rojas, *Organizers*

M. L. Auad, *Organizer, Presiding*

J. Lopez-Sanchez, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **376.** Wood-derived hemicelluloses as green binders in wood adhesives. **L. Fogelström**, E. Norström, J. Holmqvist, S. Pendergraph, J. Brücher, E.E. Malmstrom

8:30 CELL **377.** Novel thermoset polymeric networks from fast pyrolysis bio-oil. **M.L. Auad**, M. Barde, B. Sibaja

8:55 CELL **378.** Development of clay-like extrudable wood fiber material. K. Kawamura, K. Takayanagi, **H. Nonaka**

9:20 CELL **379.** Synthesis and characterization of bio-oil-based self-curing epoxy resin. **Y. Celikbag**, S. Meadows, M. Barde, S. Adhikari, G. Buschle-Diller, M. Auad, B. Via

9:45 Intermission.

10:00 CELL **380.** Valorization of starchy, cellulosic, and sugary food waste into value-added chemicals. **I. Yu**, D. Tsang

10:25 CELL **381.** Microcellular foaming of arabinoxylan with $scCO_2$. **L. Hardelin**, A. Ström, A. Larsson

10:50 CELL **382.** Transforming biomass to chemicals and fuels with light and catalysis. **J. Lopez-Sanchez**

11:15 CELL **383.** Agricultural and industrial residues: Cellulose fiber and its nanocrystals. **D. Rosa**, J. Nunes de Macedo, A. Souza

Carbohydrate-Based Nanomaterials & Drug-Delivery Vehicles

Sponsored by CARB, Cosponsored by CELL

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

WEDNESDAY AFTERNOON

Section A

Moscone Center
252/260

Bio-based Gels & Porous Materials

Biopolymer Organogels

Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Financially supported by EPNOE

T. Budtova, *Organizer*

F. Liebner, *Organizer, Presiding*

H. Mansur, *Presiding*

1:05 CELL **384.** Withdrawn.

1:30 CELL **385.** Multifunctional hydrogel dressing material for treatment of chronic wound. **I.S. Stefanov**, S. Pérez-Rafael, T. Tzanov

1:55 CELL **386.** Hierarchically porous nanocellulose materials for cartilage applications. **N. Naseri**, **A. Mathew**

2:20 CELL **387.** Cellulose-based hydrogels with encapsulative cyclooligosaccharides to enhance the efficient release of hardly soluble drugs. **D. Jeong**, S. Joo, S. Jung

2:45 Intermission.

3:00 CELL **388.** Biomass-derived highly stretchable and elastic hydrogels with effective antimicrobial activity. **Y. Si**, Z. Zheng, G. Sun

3:25 CELL **389.** Preparation of cellulose and chitin-CdTe quantum dots films and antibacterial effect on Staphylococcus aureus and Pseudomonas aeruginosa. **P. Wansapura**, N. Abidi, R. Dassanayake, A. Hamood, P. Tran

3:50 CELL **390.** Cellulose aerogels via self-assembling and electrospinning. F. Jiang, **Y. Hsieh**

4:15 CELL **391.** Nanocellulose composite hydrogels – Tailoring of mechanical properties of tissue scaffolds. **E. Heggset**, K. Syverud

Section B

Moscone Center
262

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Advanced Materials & Structures

Cosponsored by MPPG‡ and POLY

L. A. Lucia, *Organizer*

A. Ayoub, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **392.** Reactive extrusion of zein with glyoxal and polyethylene maleic anhydride. **G.W. Selling**, K. Utt

1:30 CELL **393.** Melt-processing of cellulose pulp and polycaprolactone composites: Wet feeding approach to improve the filler dispersion. **G. Lo Re**, S. Spinella, F. Vilaseca, L. Berglund

1:55 CELL **394.** Reactive extrusion compatibilization of cellulose acetate/water soluble polymer blends. **R. Quintana Vicente**, O. Persenarie, Y. Lemmouchi, L. Bonnaud, P. Dubois

2:20 CELL **395.** Reactive compatibilizers in the creation of wood fiber plastic composites. **J. Pawlak**, Y. Wang

2:45 Intermission.

3:00 CELL **396.** Liquid assisted extrusion process of cellulose nanocomposites. **K.A. Oksman**, N. Herrera, A. Singh

3:25 CELL **397.** New insights in melt processing of cellulose nanomaterial based nanocomposites. **A. Dufresne**

3:50 CELL **398.** Extrusion technology for nanocomposite containing renewable lignocellulosic materials. **R.A. Venditti**

4:15 CELL **399.** Processing of (nano) biocomposite foams by continuous supercritical CO_2 assisted extrusion. **N. Le Moigne**, M. Sauceau, M. Chauvet, M. Benyakhlef, E. Rodier, J. Fages

4:40 Concluding Remarks.

Section C

Moscone Center
270

Advances in Polysaccharides: Practice & Applications

Novel Materials & Methodologies

Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

A. Biswas, H. Cheng, *Organizers*

W. J. Orts, *Presiding*

1:05 CELL **400.** Polysaccharide-surfactant association—basics and applications. **B. Lindman**, T. Nylander, M. Miguel, F. Antunes, F. Cuomo

1:30 CELL **401.** Creating cost-effective agriculturally-derived nanocomposites for commodity applications. **W.J. Orts**, G.H. Tonoli, G.M. Glenn, K.M. Holtman, L.F. Torres, D.F. Wood

1:55 CELL **402.** Functional cellulosic arabinoxylan fiber from agricultural biomass. **M.P. Yadav**, R. Moreau, K.B. Hicks, M. Kale

2:20 CELL **403.** Strategies toward cellulose nanofibers, porous fibers and hybrids. **Y. Hsieh**

2:45 Intermission.

3:00 CELL **404.** UV-absorbing materials based on natural molecular sunscreens and chitosan. S.C. Fernandes, **V. Bulone**

3:25 CELL **405.** Higher value films prepared from poly(vinyl alcohol) and amylose-fatty acid derivatives inclusion complexes. **G.W. Selling**, G. Fanta, F.C. Felker, W.T. Hay

3:50 CELL **406.** Bio-based sources for *p*-xylene. **P.B. Smith**, D.R. Henton, A. Dumitrascu, D.A. Hucul, M. Masuno, R. Smith, J. Bissell

4:15 CELL **407.** Chemical platform for the production of Bio-PET. **R. Smith**

Section D

Moscone Center
272

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Cosponsored by AGFD, ANYL and POLY

Financially supported by HORIBA Instruments Incorporated; University of Tokyo, Japan; Innventia AB; U.S. Forest Service

U. P. Agarwal, T. J. Elder, A. Isogai, T. Larsson, *Organizers*

M. G. Laborie, N. Robitaille Brown, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **408.** Single-sourced nanocelluloses: Process-linked characteristics and behaviors. **Y. Hsieh**

1:30 CELL **409.** Interactions betwen cellulose and random and block copolymers: Antifouling and friction. M. Vuoriluoto, H. Orelma, L. Johansson, **O.J. Rojas**

1:55 CELL **410.** Conformational energy distribution for crystals of cellobiose and analogs. **A.D. French**

2:20 CELL **411.** Three-dimensional alignment of lamella single crystals of cellulose II using magnetic field. **M. Wada**, S. Wakiya, K. Kobayashi, S. Kimura, M. Kitaoka, R. Kusumi, F. Kimura, T. Kimura

2:45 Intermission.

3:00 CELL **412.** New model for untangling cellulose ultrastructure. **U.P. Agarwal**

3:25 CELL **413.** Dynamic FTIR as a tool to assess the interaction of lignin in wood pulps. **L. Salmén**

3:50 CELL **414.** Modeling the mesoscale architecture of lignocellulose to elucidate its impact on transport phenomena and biomass conversion processes. **P.N. Ciesielski**, M.F. Crowley, B.S. Donohoe, M. Himmel

4:15 CELL **415.** Chemical microscopy of polysaccharide surfaces using TOF-SIMS. **P.E. Fardim**

Section E

Moscone Center
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Functional Lignocellulosics & Nanotechnology

Responsive Materials & Biosensors

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, T. Nypelo, M. S. Peresin, *Organizers*

E. Filpponen, S. Spirk, *Organizers*, *Presiding*

1:05 CELL **416.** Investigation of the thermodynamics of the interaction of (modified) cellulose nanocrystals with natural polymers. **W. Thielemans**

1:30 CELL **417.** Cellulose-inorganic hybrid structures as promising thermoelectric materials. **T. Tammelin**, M. Gestranius, M. Putkonen, B.P. Wilson, M. Karppinen, E. Kontturi

1:55 CELL **418.** Nanocellulose mediated layer-by-layer chip modification for cellular *in-vitro* diagnostics. **T. Pettersson**, H. Ramachandraiah, A. Russom

2:20 CELL **419.** Multi-layered polysaccharide based nanofilms for the treatment of chronic venous ulceration. J. Stana, J. Stergar, L. Gradišnik, R. Kargl, V. Flis, T. Mohan, **K. Stana Kleinschek**, U. Maver

2:45 Intermission.

3:00 CELL **420.** Graft modification of cellulose nanocrystals with carbon dioxide responsive polymers via living radical polymerization. O. Garcia-Valdez, J. Arredondo, P.G. Jessop, P. Champagne, J. Bouchard, **M.F. Cunningham**

3:25 CELL **421.** Quantitative modelling of water transport in ultrathin cellulose nanofibril films. **M. Hakalahti**, E. Kontturi, T. Tammelin

3:50 CELL **422.** Impact of water vapor adsorption on physically treated cellulose thin films. **D. Reishofer**, R. Resel, G. Drexler, W. Fischer, T. Tammelin, E. Kontturi, **S. Spirk**

4:15 CELL **423.** Elaboration of cellulose nanocrystals CNC/Ge-imogolites multilayered thin films. **C. Mauroy**, C. Levard, C. Moreau, B. Cathala, J. Rose

Section F

Moscone Center
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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

M. L. Auad, O. J. Rojas, *Organizers*

J. Campos-Teran, *Organizer, Presiding*

G. Toriz Gonzalez, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **424.** Alkylation of unsaturated fatty compounds.

1:30 CELL **425.** Valorization of industrial biomass ash in structural materials. **H. Uvegi**, P. Chaunsali, R. Osmundsen, J. Ochsendorf, E. Olivetti

1:55 CELL **426.** Adsorption and viscoelastic studies of gold Nanoparticles (NPAu) and Bovine Serum Albumin (BSA) complexes at chitosan-alginate-cellulose films. D. Gómez-Maldonado, R. López-Simeon, A. Topete, **J. Campos-Teran**

2:20 CELL **427.** Sustainable hybrid bio-composites for automotive applications. **A. Rodriguez Uribe**, S. Vivekanandhan, M. Misra, A. Mohanty

2:45 Intermission.

3:00 CELL **428.** Reactive film-forming maleimido dextrans for cysteine-containing surfaces adsorbing BSA. T. Elschner, F. Obst, T.J. Heinze, **R. Kargl**, K. Stana Kleinschek

3:25 CELL **429.** Morphological and thermo-chemical changes upon autohydrolysis and microemulsion treatments of coir and EFB residual biomass to isolate lignin-rich Micro and Nano Fibrillar Cellulose (MNFC). **A. Tripathi**, A. Ferrer, S.A. Khan, O.J. Rojas

3:50 CELL **430.** Effect of cellulose nanofibril morphology on the strength and stiffness of macroscopic filaments. **N. Mittal**, T. Kaldeus, F. Lundell, D. Soderberg

4:15 CELL **431.** Role of lignin on functional and physicochemical properties of enzymatic modified soy protein film. **E. Zadeh**, Y. Kim

Section G

Moscone Center
130

Frontiers in Glycoanalytics

MS & NMR Methods

Cosponsored by ANYL, CARB‡ and MPPG‡

Financially supported by Agilent Technologies; Bruker BioSpin Corporation; Postnova Analytics, Incorporated; Rigaku Corporation; Waters Corporation; Wyatt Technology Corporation

G. Boons, M. Roman, *Organizers*, *Presiding*

1:10 Introductory Remarks.

1:15 CELL **432.** MS techniques in structure analysis of complex glycans. **F. Vilaplana**, A. Martínez-Abad, A. Ruthes

1:55 CELL **433.** Advancing glycopeptide characterization using high sensitivity HILIC-MS methods. **W. Alley**, Y. Yu, M. Lauber

2:20 CELL **434.** Infrared spectroscopy integrated to mass spectrometry: An innovative platform for *de novo* carbohydrate sequencing. **I. Compagnon**

2:45 Intermission.

3:00 CELL **435.** Examining glycan structure and dynamics with NMR: A tutorial. **J.H. Prestegard**

3:40 CELL **436.** Asparagine-linked glycosylation of immunoglobulin G and the Fc gamma receptors impacts immune system activation. **A.W. Barb**

4:05 CELL **437.** NMR Analysis of substituent distribution in polysaccharide derivatives. **S. Liu**, K.J. Edgar

4:30 CELL **438.** Solid-state NMR methods to determine glycan structure, intermolecular interactions and protein binding in plant cell walls. **T. Wang**, P. Phyo, Y. Chen, D. Cosgrove, M. Hong

Carbohydrate-Based Nanomaterials & Drug-Delivery Vehicles

Sponsored by CARB, Cosponsored by CELL

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

THURSDAY MORNING

Section A

Moscone Center
252/260

Bio-based Gels & Porous Materials

Aero-, Cryo- & Xerogels

Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Financially supported by EPNOE

F. Liebner, *Organizer*

T. Budtova, *Organizer, Presiding*

C. Freire, *Presiding*

8:05 CELL **439.** Cellulose nanofiber - towards tailored release of small molecules. **A. Svagan**, L. Wagberg, J. Wohlert, A. Mullertz, D. Bar shalom, K. Löbmann

8:30 CELL **440.** Nanocellulose aerogels with thermal superinsulating properties obtained by spray freeze-drying. C. Jiménez-Saelices, B. Saentier, **B. Cathala**, Y. Grohens

8:55 CELL **441.** Anisotropic cellulose ester aerogels with tunable mechanical properties via controlled solvent exchange. **A. Tripathi**, S.A. Khan, O.J. Rojas

9:20 CELL **442.** 2,3-Dicarboxyl nano cellulose: A novel source material for transparent, birefringent and thermally superinsulating aerogels. S. Plappert, J. Nedelec, **F. Liebner**

9:45 Intermission.

10:00 CELL **443.** Functional aerogels based on nanocellulose and platinum nanoparticles/graphene oxide for catalytic applications. R. Pinto, A.A. Silvestre, M. Simões, P. Marques, **C. Freire**

10:25 CELL **444.** Fabrication of functionalized aerogels from cellulose and whole biomass for absorbing formaldehyde from indoor air. **Y. Liao**, X. Pan

10:50 CELL **445.** Superhydrophobic nanocellulose-silica composite aerogels for efficient water-in-oil emulsions separation. **S. Zhou**, F. Xu

11:15 CELL **446.** Cellulose Aerogel Reinforced Polymers (CARPs). **M. Schestakow**, L. Ratke

Section B

Moscone Center
262

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Commercial & Versatile Technology

Cosponsored by MPPG‡ and POLY

L. A. Lucia, *Organizer*

A. Ayoub, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CELL **447.** Twin-screw extrusion: A versatile tool for the pretreatment of biomass. **A. Rouilly**, V. VanDenBossche, P. Evon, M. Rigal

8:30 CELL **448.** Using reactive extrusion to manufacture greener products – from laboratory fundamentals to commercial scale. **R. Narayan**

9:20 CELL **449.** Extrusion of protein plastics. **M.S. Hedenqvist**, E. Johansson, W. Newson, M. Gällstedt, R. Kuktaite, H. Ullsten, H. Türe

9:45 Intermission.

10:00 CELL **450.** Silicone-based cellulose materials: Processes & characterizations. **E. Fleury**, C. Barres, A. Rachini, X. Zhou, J. Bernard, S. Deng, A. Charlot

10:25 CELL **451.** Withdrawn.

10:50 CELL **452.** Thermomechanical extrusion preteatment for production of ethanol and arabinoxylan from corn fiber. **G. Ryu**

11:15 CELL **453.** Optimizing high shear and other process parameters for reactive mixing and nanocomposite dispersion. **A. Farahanchi**, B. Calderon, J. Gug, M.J. Sobkowicz

11:40 Concluding Remarks.

Section C

Moscone Center
270

Advances in Polysaccharides: Practice & Applications

New Functional Materials

Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

H. Cheng, *Organizer*

A. Biswas, *Organizer, Presiding*

8:05 CELL **454.** Design of new functional polysaccharide nanoparticles for biomedical imaging applications. **M. Bozic**, M. Bracic, R. Kargl, U. Jančič, D. Tkaucic, T. Elschner, S. Hribernik, T. Mohan, K. Stana Kleinschek

8:30 CELL **455.** Chitin-Glucan nanopapers from fungi in membrane and water treatment operations. **A. Mautner**, N. Yousefi, W. Wan Nawawi, A. Bismarck

8:55 CELL **456.** Cellulose functional materials with multiple stimuli responsive and their applications in sensors. **H. Kang**, P. Li, R. Liu, Y. Huang

9:20 CELL **457.** Adsorption of IgG antibodies on cellulose thin film surface. **V. Raghuwanshi**, Z. Huang, G. Garnier

9:45 Intermission.

10:00 CELL **458.** Development of cellulose helicoidal architectures in nature. **S. Vignolini**

10:25 CELL **459.** Free-standing multilayered membranes from renewable polymers, towards tissue engineering applications. **M.P. Sousa**, F. Cleymand, J.F. Mano

10:50 CELL **460.** Structural features of polycarboxylic acids as cross-linking agents of cellulose. **G. Sun**, C. Zhao, H. Qi, B. Ji, K. Yan

11:15 CELL **461.** PEGylation of chitosan via nitroxide chemistry in aqueous media. O. Garcia-Valdez, A. Darabi, M.F. Cunningham, **P. Champagne**

Section D

Moscone Center
272

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Cosponsored by AGFD, ANYL and POLY

Financially supported by HORIBA Instruments Incorporated; University of Tokyo, Japan; Innventia AB; U.S. Forest Service

U. P. Agarwal, T. J. Elder, A. Isogai, *Organizers*

T. Larsson, *Organizer, Presiding*

Y. Hsieh, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **462.** New development of wood chemistry promoted by TOF-SIMS. D. Aoki, Y. Matsushita, K. Kuroda, **K. Fukushima**

8:30 CELL **463.** Following in-situ hydrophobisation of plant cell walls by Raman imaging. **N. Gierlinger**, B. Prats-Mateu, M. Felhofer, P. Bock

8:55 CELL **464.** On the mechanisms of cellulose dissolution in aqueous media. **B. Lindman**, B. Medronho, L. Alves, M. Norgren, H. Edlund

9:20 CELL **465.** Construction of cellulose based nanofibrous materials via green route. **L. Zhang**

9:45 Intermission.

10:00 CELL **466.** Polymerization of cellulose and lignin on a chip: Morphological studies. **N. Robitaille Brown**, S. Basu, O. Omadjela, C. Anderson, Y. Zhu, J.M. Catchmark, J. Zimmer

10:25 CELL **467.** Crystal deformation and transformation of cellulose allomorphs derived from stability of molecular chain sheets. T. Uto, **T. Yui**

10:50 CELL **468.** Imaging mass spectrometry analysis of woody cell wall using $^{13}CO_2$ pulse labeling. **M. Takeuchi**, M. Norisada, A. Isogai

11:15 CELL **469.** Withdrawn.

Section E

Moscone Center
274

Functional Lignocellulosics & Nanotechnology

‡ *Cooperative Cosponsorship*

Responsive Materials & Biosensors

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, T. Nypelo, M. S. Peresin, *Organizers*

E. Filpponen, S. Spirk, *Organizers*, *Presiding*

8:05 CELL **470.** First steps towards bio-based static true volumetric 3D displays: Transparent cellulose scaffolds equipped with photon upconverting rare earth metal doped nanophosphors (uc-NP). **S. Quraishi**, S. Plappert, T. Rosenau, F. Liebner

8:30 CELL **471.** Phase separated bicomponent biopolymer thin films - enzymatic patterning and protein interaction. **K. Niegelhell**, M. Süßenbacher, K. Jammernegg, T. Ganner, D. Schwendenwein, H. Schwab, F. Stelzer, H. Plank, **S. Spirk**

8:55 CELL **472.** Dye functionalized polysaccharide nanoparticles – From synthesis to bio-sensor applications in immunoassays. **P. Schulze**, M. Gericke, F. Scholz, P. Miethe, T.J. Heinze

9:20 CELL **473.** Cellulose-based microcapsules: Bio-compatible vessels for packing, delivery and attachment of active species. **S. Hribernik**, T. Kos, M. Kurecic, K. Stana Kleinschek

9:45 Intermission.

10:00 CELL **474.** Withdrawn.

10:25 CELL **475.** Cellulose as a template for generation, wireless transport and storage of electrical energy with conducting polymers. **S. Malti**

10:50 CELL **476.** Bacterial nanocellulose-based composites as ion exchange membranes for fuel cells. **C. Vilela**, A.A. Silvestre, F.M. Figueiredo, C.S. Freire

11:15 CELL **477.** Hydrogen bonding and polymer adsorption: A look at polyethylene glycol with cellulose and silica colloids. **M.S. Reid**, H.S. Marway, M. Villalobos, E.D. Cranston

Section F

Moscone Center

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

J. Campos-Teran, O. J. Rojas, *Organizers*

M. L. Auad, *Organizer, Presiding*

R. L. Quirino, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **478.** Activated polysaccharide nanoparticles derived from xylan phenyl carbonates – From synthesis to applications. **M. Gericke**, L. Gabriel, K. Geitel, P. Trivedi, P.E. Fardim, T.J. Heinze

8:30 CELL **479.** Emulsion polymerization of tung oil-based latexes with asolectin as a biorenewable surfactant. A. Johns, K. Edwards, S. Inglesby, **R.L. Quirino**

8:55 CELL **480.** Bioactive nano-coatings from hyaluronic acid and a lysine-derived surfactant. M. Bracic, L. Fras-Zemljič, K. Kogej, **R. Kargl**, K. Stana Kleinschek, T. Mohan

9:20 CELL **481.** Biomaterials based on polysaccharide conjugates. **R. Kargl**, A. Dobaj Štiglic, T. Mohan, U. Maver, L. Gradišnik, T. Elschner, K. Stana Kleinschek

9:45 Intermission.

10:00 CELL **482.** Green approaches to preparation of amphiphilic soy protein microfibrils and films. **X. Liu**, Y. Hsieh

10:25 CELL **483.** Improvement of BC production by a new reclassified acid-resistant strain using food supply chain waste in a two-stage fermentation. **C.A. Molina**, C. Castro Herazo, R. Zuluaga Gallego, P. Gañán

10:50 CELL **484.** Withdrawn.

Section G

Moscone Center

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Frontiers in Glycoanalytics

Molar Mass & Crystallinity Analyses

Cosponsored by ANYL, CARB‡ and MPPG‡

Financially supported by Agilent Technologies; Bruker BioSpin Corporation; Postnova Analytics, Incorporated; Rigaku Corporation; Waters Corporation; Wyatt Technology Corporation

G. Boons, *Organizer*

M. Roman, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 CELL **485.** Separation and characterization of polysaccharides by multi-detection size-exclusion chromatography and field-flow fractionation techniques. **L. Pitkanen**, A.M. Striegel

8:55 CELL **486.** Determination of thickness, aspect ratio and size distribution of cellulose nanocrystals using asymmetric flow FFF and MALS. **S. Tadjiki**, R. Reed, M. Roman

9:20 CELL **487.** Benefits of MALS, FFF and Viscometry in the characterization of polysaccharide molar mass, size, conformation and branching ratios. **J.A. Ahlgren**

9:45 Intermission.

10:00 CELL **488.** Quantitating cellulose crystallinity: Approaches, problems, and perspectives. **W.T. Winter**

10:40 CELL **489.** Simplified studies of cellulose crystallinity with a Rietveld program. **A.D. French**

11:05 CELL **490.** Vibrational spectroscopy study of crystalline cellulose – peak assignment, crystallinity, and non-linear optical responses. **S.H. Kim**

11:30 CELL **491.** Raman spectroscopy in the analysis of cellulose: Addressing the issues of crystallinity, polymorphy, and ultra-structure. **U.P. Agarwal**

THURSDAY AFTERNOON

Section A

Moscone Center

252/260

Bio-based Gels & Porous Materials

Open-Porous Carbon Materials

Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Financially supported by EPNOE

T. Budtova, F. Liebner, *Organizers*

B. Cathala, *Presiding*

1:05 CELL **492.** Nanocellulose aerogel beads: Structurable and printable energy storage. **J. Erlandsson**, H. Granberg, M. Sandberg, L. Wagberg

1:30 CELL **493.** 3D interdigitated energy storage devices built inside aerogels using layer by layer assembly. **Z. Wang**, M. Hamedi, L. Wagberg

1:55 CELL **494.** Processing and properties of elastomer covalently bound to nanocellulose aerogel. M. Fumagalli, S. Boisseau, **L. Heux**

2:20 CELL **495.** Functional polysaccharide hydrogels through chemical derivatization of agarose. **M. Gericke**, M. Witzler, M. Schulze, T.J. Heinze

2:45 Intermission.

3:00 CELL **496.** Withdrawn.

3:25 CELL **497.** Biologically modified lignin for water purification. **I. Brzonova**, C.J. Buelke, E.I. Kozliak, Y. Ji

3:50 CELL **498.** Preparation of carbon aerogels from TEMPO-oxidized cellulose nanofibers for organic solvents absorption. **M. Wang**

4:15 CELL **499.** Value-Added biomaterials from lignocellulose based on biorefinery scenario. **R. Sun**

4:40 Concluding Remarks.

Section B

Moscone Center

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Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Energy, Food & Packaging Development

Cosponsored by MPPG‡ and POLY

L. A. Lucia, *Organizer*

A. Ayoub, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **500.** Melt extrusion of lignin carbon-fiber precursors: The path forward for low-cost fibers or unrealizable dream? **D.P. Harper**, O. Hosseinaei

1:30 CELL **501.** Melt extrusion of acrylonitrile based quad-polymer precursor for green carbon fiber technology. **S. Mahmood**, B.L. Batchelor, M. Jung, H. Song, D. Yang

1:55 CELL **502.** Rheology and modeling of complex food systems in reactive extrusion. **M. Emin**, H. Schuchmann

2:20 CELL **503.** Polymerization of sugars by reactive twin-screw extrusion to produce soluble fibers for food and feed. **T.C. Schoenfuss**, A. Kuechel, C. Tyl

2:45 Intermission.

3:00 CELL **504.** Advanced thermal analysis modelling for the characterization of active poly(lactic acid)/natural fibre food-packaging composite materials. **S.W. Bigger**, M.J. Cran, I.S. Tawakkal

3:25 CELL **505.** Utilization of coffee wastes in biobased composite materials for food packaging uses. **T. Wang**, N. Zarrinbakhsh, R. Muthuraj, A. Rodriguez-Uribe, S. Vivekanandhan, M. Misra, A. Mohanty

3:50 CELL **506.** Withdrawn.

4:15 CELL **507.** Preparation of water soluble oligosaccharides from sugar reversion reactions in acidic lithium bromide trihydrate. **N. Li**, X. Pan

4:40 Concluding Remarks.

Section C

Moscone Center

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Advances in Polysaccharides: Practice & Applications

Preparation, Characterization & Applications

Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

A. Biswas, H. Cheng, *Organizers*

H. Cheng, R. Furtado, *Presiding*

1:05 CELL **508.** Gradient separations and two-dimensional separations of cellulose derivatives. **W. Radke**

1:30 CELL **509.** New insight into the gelation of Na-alginate aqueous solution. **R. Liu**, C. Zhao, K. Sui, Y. Xia

1:55 CELL **510.** Electrospun polysaccharide based materials as modern wound dressings. **M. Kurečič**, U. Maver, T. Maver, T. Pivec, T. Rijavec, A. Lapanje, S. Hribernik, K. Stana Kleinschek

2:20 CELL **511.** Hemicelluloses cationization: Comparison of liquid and solid phase preparation processes. **D. Da Silva Perez**, V. Bigand, C. Pinel, F. Rataboul, M. Petit-Conil

2:45 Intermission.

3:00 CELL **512.** Use of polysaccharides from cashew gum in encapsulation applications. **R. Furtado**, L.C. Silva, M.A. Nascimento, L.G. Mendes, T.L. Barroso, G.A. Freire

3:25 CELL **513.** Electrosynthesis and characterization of polypyrrole/cashew gum composite. R. Furtado, J.R. Maciel, M. Oliveira, **C.R. Alves**

3:50 CELL **514.** Novel polyurethanes from Xylan and TDI: Preparation and characterization. **H. Cheng**, A. Biswas

4:15 Concluding Remarks.

Section D

Moscone Center

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Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Cosponsored by AGFD, ANYL and POLY

Financially supported by HORIBA Instruments Incorporated; University of Tokyo, Japan; Innventia AB; U.S. Forest Service

U. P. Agarwal, T. J. Elder, T. Larsson, *Organizers*

A. Isogai, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CELL **515.** In situ Raman Microscopy to monitor changes in cellulose crystallinity during acid pre-treatment. **M.T. Timko**

1:30 CELL **516.** On the ionization of cellulose in aqueous alkali. **D. Bernin**, E. Bialik, B. Stenqvist, Y. Fang, Å. Östlund, I. Furo, B. Lindman, M. Lund

1:55 CELL **517.** Structural factors affecting ^{13}C NMR chemical shifts of C4 and C6 of cellulose – a computational study. **H. Yang**, T. Wang, D. Oehme, L. Petridis, M. Hong, J.D. Kubicki

2:20 CELL **518.** Effect of dilution-freezing-drying process on Cellulose Nanocrystals (CNCs) for Polylactic Acid (PLA)-CNC composite packaging. **N. Stark**, R. Sabo, L. Wei, R. Reiner, A. Rudie

2:45 Intermission.

3:00 CELL **519.** Liquids NMR toolbox for the analysis of modified nanocelluloses. **A. King**, T. Laaksonen, S.A. Kedzior, A.J. Holding, J.K. Helminen, S. Heikkinen, V. Mäkelä, E.D. Cranston, I. Kilpeläinen

3:25 CELL **520.** In-situ visualization of structural changes to biomass during chemical reactions using neutron scattering. **S. Pingali**, H.M. O'Neill, V. Urban, L. Petridis, B. Evans, J. Smith, P. Langan, B.H. Davison

3:50 CELL **521.** Recovery of high-purity levoglucosan and other anhydrosugars from pyrolysis oil. **M.R. Rover**, P.H. Hall, J. Stanford, P. Johnston, R.G. Smith, R.C. Brown

4:15 CELL **522.** Probing the dehydration induced changes in the organization of cellulose microfibrils in primary cell walls using Sum-Frequency-Generation (SFG) vibrational spectroscopy. **S. Huang**, Y. Zheng, S. Kiemle, D. Cosgrove, S.H. Kim

Section E

Moscone Center

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Functional Lignocellulosics & Nanotechnology

(nano)Paper: From Fundamentals to Applications/Antimicrobial, Functional Materials

Cosponsored by CARB and COLL

Financially supported by EPNOE

M. K. Ek, E. Filpponen, T. Nypelo, M. S. Peresin, *Organizers*

S. Spirk, *Organizer, Presiding*

W. Fischer, *Presiding*

1:05 CELL **523.** Microfluidic paper - influence of fiber source, sheet properties and fiber surface modification on capillary driven flow. **M.A. Biesalski**, A. Böhm, S. Wendenburg

1:30 CELL **524.** Combined mechanical and chemical modifications towards super-stretchable paper-based materials. **A. Khakalo**, J. Kouko, I. Filpponen, E. Retulainen, O.J. Rojas

1:55 CELL **525.** Fiber fines – Properties and influence of cellulosic microparticles. **W. Fischer**, R. Schmiedt, L.A. Jagiello, M. Mayr, R. Giner Tovar, S. Spirk, R. Eckhart, W. Bauer

2:20 CELL **526.** Utilization of polymerized technical lignins in the development of surface sizing formulations for packaging papers. **S. Kopacic**, A. Ortner, G.M. Guebitz, W. Bauer, K. Mahler, K. Hofer, K. Eibinger, T. Kraschitzer

2:45 Intermission.

3:00 CELL **527.** Layer-by-layer modification of cellulosic materials for green antibacterial materials. A. Ottenhall, C. Chen, J. Henschen, J. Illergård, P.A. Larsson, L. Wagberg, **M.K. Ek**

3:25 CELL **528.** Purification of water using cellulose: A safe way to remove bacteria. **A. Ottenhall**, T. Seppänen, M.K. Ek

3:50 CELL **529.** Evaluation of Antibacterial functionalizations of CNF/PVAm multilayer modified cellulose fibre and surface studies on silica model surface. **C. Chen**, J. Illergård, L. Wagberg, M.K. Ek

4:15 CELL **530.** Film formation and performance of different nanocelluloses obtained from different cellulose sources after different preparation processes. **Y. Zhao**, C. Moser, M.E. Lindström, G. Henriksson, **J. Li**

Section F

Moscone Center

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Valorization of Renewable Resources & Residuals into New Materials & Multiphase Systems

Cosponsored by AGFD

M. L. Auad, J. Campos-Teran, *Organizers*

O. J. Rojas, *Organizer, Presiding*

A. Villares, *Presiding*

1:00 Introductory Remarks.

1:05 CELL **531.** Cellulose nanofibrils in emulsions stabilized by an ionic surfactant and effect of electrolyte in phase transitions. S. Huan, S. Yokota, M. Ago, M. Borghei, T. Kondo, **O.J. Rojas**

1:30 CELL **532.** *In situ* biomineralization of hydroxyapatite on bacterial nanocellulose and use as bioink for 3D bioprinting scaffolds to engineer bone. **G. Toriz Gonzalez**, P. Gatenholm

1:55 CELL **533.** Deep Eutectic Solvent (DES) treatment in nanofibrillation of secondary cellulose raw materials. **T.T. Suopajärvi**, J.A. Sirviö, H. Liimatainen

2:20 CELL **534.** Oil in water Pickering emulsions stabilized by cellulose nanocrystals-xyloglucan complexes. **A. Villares**, Z. Jaafar, C. Moreau, I. Capron, B. Cathala

2:45 Intermission.

3:00 CELL **535.** Water-based bentonite fluids modified by cellulose nanoparticles for minimizing fluid loss and formation damage. **Q. Wu**

3:25 CELL **536.** Mechanical isolation of nanocellulose from paper industry waste by ball mining. **D. Rosa**, F. Kano, A. Souza

3:50 CELL **537.** Chemical isolation and characterization of cellulose nanofibers to produce bionanocomposite films onto chitosan matrix for seafood packaging. **B. Soni**

‡ *Cooperative Cosponsorship*

CHED

Division of Chemical Education

T. Miller, *I. Levy and C. Muzzi, Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences (see *ENVR*, Mon, Wed)

Processes, Technologies & Sensors for Food-Energy-Water Nexus Research (see *ENVR*, Tue)

SOCIAL EVENTS:

High School-College Interface Luncheon (Tickets required), 12:00 PM: Sun

CHED Division Reception, 5:30 PM: Sun

SUNDAY MORNING

Section A

San Francisco Marriott Marquis

Golden Gate C2

High School Program

Cosponsored by WCC

S. B. Mitchell, *Organizer*

J. L. Ball, *Organizer, Presiding*

8:00 Registration.

8:30 Introductory Remarks.

8:35 CHED **1.** Teaching chemistry today with an environmentally responsible view of tomorrow. **B.H. Lipshutz**

9:05 Intermission.

9:15 CHED **2.** Middleschoolchemistry.com lesson shows that carbon dioxide can make water acidic. **J. Kessler**

9:55 CHED **3.** Reconstructing ancient human diet in the prehistoric San Francisco Bay area using stable isotopes: Building data sets and careers through student collaboration. **E.J. Bartelink**

10:25 CHED **4.** Who asks a more beautiful question. **J. Hubbard**

10:55 Concluding Remarks.

Section B

San Francisco Marriott Marquis

Salons 3/4

State of the Art: Applying Chemistry Education Research to Practice

D. G. Herrington, *Organizer*

P. L. Daubenmire, *Organizer, Presiding*

8:30 CHED **5.** Who are the chemistry students we serve these days? **P.L. Daubenmire**, D.G. Herrington

8:50 CHED **6.** Learning in context: Research evidence and chemistry education practice. **P.G. Mahaffy**

9:30 CHED **7.** Fostering student learning of chemistry through metacognition: Linking current metacognitive research with practice. **M.T. Dianovsky**

10:10 Intermission.

10:25 CHED **8.** Applying CER and domain-general research to create an intimate learning environment in large lecture courses. **E.J. Yezierski**

11:05 CHED **9.** Implementation and evaluation of screencasts and simulations for online learning. **R.D. Sweeder**, **J.R. Vandenplas**, D.G. Herrington

11:45 CHED **10.** OrgChem101.com: Online learning modules that can be used in blended, flipped, traditional, or other classroom environments. **A.B. Flynn**, R.E. Featherstone, N. Bodé, J. Caron, J. Laroche, M. Bélanger, G. Richard, R. Visser

Section C

San Francisco Marriott Marquis

Salon 5

Citizens First!

Cosponsored by CEI

R. D. Sheardy, *Organizer*

C. Maguire, *Organizer, Presiding*

K. Slavens, *Presiding*

8:30 Introductory Remarks.

8:40 CHED **11.** New Chemistry in Context: The chemistry of portable electronics. **J.S. Kirk**

9:00 CHED **12.** Citizens first in the laboratory. **J.A. Tripp**, L.C. McKenzie

9:20 CHED **13.** Connecting chemistry to community with deliberative democracy. **R. Komperda**, L. Griffith, E. Olsen, K. Hosbein, C. Zografos, J. Barbera, E. Shortlidge, G.P. Shusterman

9:40 CHED **14.** Evaluating the economic viability of a copper mine in the first-year chemistry laboratory using visible spectroscopy. **A.P. Bopegedera**

10:00 Intermission.

10:15 CHED **15.** Achieving civic engagement by integrating real research into a general education chemistry course. **W.R. Midden**

10:35 CHED **16.** Flipping the non-science majors chemistry course – No, not that type of flipping: Chemical weapons and a relevant-issues driven chemistry course. **M.A. Bishop**

10:55 CHED **17.** Learning to cross boundaries. **S. Glazier**, E. Metzger

11:15 CHED **18.** Soap, detergents, and personal care products. **D.A. Katz**

11:35 Concluding Remarks.

Section D

San Francisco Marriott Marquis

Salon 6

Green Chemistry: Theory & Practice

Cosponsored by CEI

Financially supported by I&EC Green Chemistry; Green Chemistry Institute

J. E. Wissinger, *Organizer*

E. J. Brush, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **19.** Improved greener synthesis of thiosemicarbazones. **N. Rosenfeld**, J. Bennett

8:55 CHED **20.** Synthesis of dilantin using green chemistry. **V. Sublett**, D.J. Swartling

9:15 CHED **21.** Changes in the green and sustainable chemistry undergraduate curriculum at GVSU. **D.G. Kovacs**

9:35 Intermission.

9:50 CHED **22.** Development of an assessment tool to measure student proficiency in green chemistry concepts and skills. **L. Armstrong**, G. Kerstiens, M.T. Robak, M.C. Douskey, A.M. Baranger

10:10 CHED **23.** Enhancing the next generation of green scientists. **D. Paull**

10:30 CHED **24.** Models for integrating toxicology into chemistry courses. A.S. Cannon, **A. McCarthy**

10:50 CHED **25.** Fundamentals and challenges for a sustainable chemical enterprise. **M. Sabahi**, E. Reichmanis

Section E

San Francisco Marriott Marquis

Nob Hill A

Research in Chemistry Education

New & Noteworthy in 2015-2016

D. P. Cartrette, D. R. Mulford, *Organizers*

G. T. Rushton, M. N. Stains, M. Teichert, J. Walker, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **26.** Biochemistry instructors' perceptions of analogies and their classroom use. **M. Orgill**, T.J. Bussey, G.M. Bodner

9:15 CHED **27.** Affective learning and organic chemistry achievement: Testing models of reciprocal causation. **J.R. Raker**, S. Villafañe, X. Xu

9:55 Intermission.

10:10 CHED **28.** Using digital badges for assessment of hands-on skills in the laboratory. **M.H. Towns**, S. Hensiek, C.J. Harwood, B. DeKorver, J. Fish

10:50 CHED **29.** Improving critical thinking via authenticity: The CASPiE research experience in a military academy chemistry course. **A. Chase**, H. Clancy, R.P. Lachance, B. Mathison, M. Chiu, G.C. Weaver, D. Sears, J.E. Dietz

11:30 Concluding Remarks.

Section F

San Francisco Marriott Marquis

Nob Hill B

NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Bruker; ThermoFisher Scientific; JEOL; Anasazi Instruments

L. J. Anna, D. P. Soulsby, A. S. Wallner, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **30.** Practical use of ^{13}C benchtop NMR spectroscopy in an undergraduate laboratory. **P.J. Bowyer**, B. Manz, A. Coy, H. Robert

8:55 CHED **31.** Hands-on NMR experience without the NMR: Using MestreNova to teach an undergraduate organic structure elucidation course without an on-site high field NMR. **K.N. Maloney**

9:15 CHED **32.** NMR spectroscopy and complementary computational tools: Delta for 1D processing, ChemDoodle for predictions, and ChemSpider for interactive literature spectra. **J. Bennett**

9:35 Intermission.

9:50 CHED **33.** Withdrawn.

10:10 CHED **34.** Biochemical NMR spectroscopy course for upper level undergraduates that combines both classroom and laboratory learning. **B.J. Stockman**

10:30 CHED **35.** Extending ^{1}H-NMR analysis into an upper-division biochemistry course to investigate enzyme stereoselectivity and active-site architecture. **T.J. Gries**

10:50 CHED **36.** Applications of quantitative NMR in chemical education. **C. Nicholson**, R. Hill, S. Barrington

11:10 Concluding Remarks.

Section G

San Francisco Marriott Marquis

Nob Hill C

Undergraduate Research Papers

Cosponsored by SOCED

C. V. Gauthier, N. L. Snyder, *Organizers*

J. V. Ruppel, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **37.** Mechanistic studies of Niemann-Pick C1. **M.N. Trinh**, F. Lu, M.S. Brown, J.L. Goldstein

8:45 CHED **38.** Tissue-specific CRISPR/Cas9 mutants: A tool to study the role of epigenetics in stem cells. **C. Torres Caban**, A. Doi, H. Horvitz

8:55 CHED **39.** Effect of BET inhibitor in drug resistant breast cancer. **L.A. Acevedo-Soto**, S.S. Akhand, M.K. Wendt

9:05 CHED **40.** Improved radiosynthesis of 3'-deoxy-3'-[^{18}F]fluorothymidine and its *in vivo* application as a proliferation imaging marker in positron emission tomography. **A. Nguyen**, J. Mishra, Z. Visco, A.L. Vāvere, E. Butch, S.E. Snyder

9:15 Intermission.

9:30 CHED **41.** Examination of genes related to T-ALL in the 8q24 region. **J. Bautista**, R. Sieg, J. Blackburn

9:40 CHED **42.** Antimicrobial and colloidal properties of novel polycationic amphiphiles. **B. Ashamole**, E. Rogers, E. Ogunjirin, K. Seifert, K.L. Caran

9:50 CHED **43.** Study of fluorescent quaternary ammonium amphiphiles to gain insight into the mechanism of antibacterial activity. **M.K. Lauer**, E. Rogers, C. Kubow, K. Seifert, K.L. Caran

10:00 CHED **44.** Investigating antimicrobial properties of the human galectin-9. **J. Van Riper**, N. Kamili, C. Gerner-Smidt, C. Arthur, S. Stowell, A. Blenda

10:10 Intermission.

10:25 CHED **45.** Effect of glutamine and γ-glutamylglutamine on NIH-3T3 cell metabolism. **N. Kowalkowski**, R. Penney, G. Boysen

10:35 CHED **46.** CYP2C9 and the mutations that affect NSAID oxidation efficiency. **B. James**, G.P. Miller, M.D. Perry

10:45 CHED **47.** Characterization of hydrogelating nucleopeptides. **S. Schrecke**, S. Brown, J.E. Smith-Carpenter

10:55 CHED **48.** Effect of 1,2-dithiolane modifications on peptide self-assemblies. **R.R. Neves**, A. Calixte, J.E. Smith-Carpenter

11:05 Intermission.

11:20 CHED **49.** Investigating trends in DNA backbone structure and dynamics for ideal drug binding: A ^{31}P NMR study of the CRE sequence. **G. Spurzem**, M. Kyinn, A. Pincus, M.E. Hatcher

11:30 CHED **50.** Inhibitition of palmitate-induced lipotoxicity. **J. Neufeld**, A.K. Stoeckman

11:40 CHED **51.** Investigation of the effect of AuNVs conjugated with modified gp100 peptide and with modified PEG on induced IL-12 cytokine production. **Á.A. Garcés**, E. Reiser Evans, J.M. Almeida, A.Y. Lin, A. Foster, R. Drezek

11:50 CHED **52.** Towards further understanding of kinase activity during oxidative stress: Senthesid of the highly active ERK2 substrates sub-D and sub-s. **O. Tornow**, A.J. Wommack

12:00 Concluding Remarks.

Section H

San Francisco Marriott Marquis

Nob Hill D

Eye Tracking Research in Chemistry Education

J. R. Vandenplas, *Organizer*

S. J. Hansen, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **53.** Eye movement patterns in solving science ordering problems. H. Tang, **E. Day**, L.K. Kendhammer, J.N. Moore, S.A. Brown, N.J. Pienta

8:55 CHED **54.** Assessing pupillometry data using multimodel inference. **J. Karch**, J. Garcia, H. Sevian

9:15 CHED **55.** Use of scan path analysis to determine biochemistry expert-novice differences in reading metabolic pathways. **K.J. Linenberger Cortes**, K. Kammerdiener

9:35 Intermission.

9:40 CHED **56.** Impact of expertise on allocation of attention during multiple-choice problem solving. **J.R. Vandenplas**, T.C. Pentecost, J. Vogl

10:00 CHED **57.** Where did you look? **S.J. Hansen**

10:20 CHED **58.** Use of eye-tracking to aid in the articulation of visual representations. **J.J. Reed**, J.R. Raker, K.L. Murphy

10:40 CHED **59.** Using R to perform advanced analysis of eye tracking data. **H. Tang**, N.J. Pienta

11:00 Concluding Remarks.

Blending Chemistry & Culture: Undergraduate Research Abroad through ACS IREU Program

Sponsored by IAC, Cosponsored by CHED

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Sponsored by ENVR, Cosponsored by CHED

Undergraduate Symposium

Sponsored by AGFD, Cosponsored by CHED

Incorporating Polymer Science into the Classroom

Undergraduate Curriculum

Sponsored by POLY, Cosponsored by CHED, MPPG‡ and PMSE

SUNDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Golden Gate C2

High School Program

Cosponsored by WCC

S. B. Mitchell, *Organizer*

J. L. Ball, *Organizer, Presiding*

1:00 CHED **60.** Tracing the steps to the Conant Award. **D. Cullen**, G.T. Rushton

1:10 CHED **61. Award Address** (James Bryant Conant Award in High School Chemistry Teaching sponsored by the American Chemical Society). Making connections that matter! **L.E. Slocum**

1:50 CHED **62.** Deep impact: Summer research with high school students. **L.S. Ott**

2:10 CHED **63.** Designing three-dimensional assessments. **M. Cooper**

2:35 Intermission.

2:45 CHED **64.** Establishing a culture of laboratory safety in secondary education. **K.M. Lopez**

3:05 CHED **65.** Sex, drugs, and the high school chemistry curriculum. **M. Wynn**

3:35 CHED **66.** Advanced materials for corrosion prevention. **S.C. Rukes**

4:15 Concluding Remarks.

Section B

San Francisco Marriott Marquis

Salons 3/4

State of the Art: Applying Chemistry Education Research to Practice

P. L. Daubenmire, *Organizer*

D. G. Herrington, *Organizer, Presiding*

1:30 CHED **67.** Supporting students' reasoning with mathematical models through simulation-focused collaborative learning activities. **N.M. Becker**

2:10 CHED **68.** Using discourse analysis to inform the design of active learning materials. **R.S. Cole**, C. Stanford, A.C. Moon, M.H. Towns

2:50 Intermission.

3:05 CHED **69.** Incorporating research on misconceptions into the classroom through the development and use of concept inventories. **C.J. Luxford**

3:45 CHED **70.** Student assessments to measure concept retention. **S.E. Lewis**

4:25 CHED **71.** Designing and using assessments items that provide evidence about depth of understanding. **M. Cooper**

5:05 Concluding Remarks.

Section C

San Francisco Marriott Marquis
Salon 5

Citizens First!

Cosponsored by CEI

C. Maguire, *Organizer*

R. D. Sheardy, *Organizer, Presiding*

R. Bishop, *Presiding*

1:30 Introductory Remarks.

1:40 CHED **72.** Learning by doing: How and why civic engagement increases durable learning. **S. Carroll**

2:00 CHED **73.** Reaching the community through Kappa Epsilon Mu (K.E.M. Club): Teaching our students to be good citizens. **K. Slavens**

2:20 CHED **74.** TWU pioneer research at the mall. **N. Mirsaleh-Kohan**

2:40 CHED **75.** Molecules of life: Teaching chemistry in the context of biological molecules and pharmaceuticals. **T. Jordan**

3:00 Intermission.

3:15 CHED **76.** Crowd-sourced data collection in a general education physical science course reveals the value of large-scale undergraduate research to finding solutions to problems of civic and conservation importance. **R. Bishop**, P.J. Carlson, L. Robinson, H. McAlexander

3:35 CHED **77.** Impact of septic systems on Long Island's aquifer. **C.J. Foley**, N. Leonhardt, M. Altizer-Evans, N. Niemann, E. Merenda

3:55 CHED **78.** Combining chemistry with knowledge of the local environment. **L.K. Duffy**, C.H. Middlecamp, L. Nicholas-Figueroa, T.D. Lindstrom, K. Dunlap

4:15 CHED **79.** Relevent learning in science education: Research, development and implimentation. **M. Hugerat**

4:35 Concluding Remarks.

Section D

San Francisco Marriott Marquis
Salon 6

Green Chemistry: Theory & Practice

Cosponsored by CEI

Financially supported by I&EC Green Chemistry; Green Chemistry Institute

E. J. Brush, *Organizer*

J. E. Wissinger, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **80.** Green chemistry = social and environmental justice. **E.J. Brush**

1:55 CHED **81.** Environmental justice, sustainability and green chemistry. **L. Bastin**

2:15 CHED **82.** Science for social change: A first-year interest group incorporating green chemistry and environmental justice principles. **D.H. Exton**

2:35 Intermission.

2:50 CHED **83.** How student chapters can have impact on green chemistry and social justice education. **V. Curfman**, **I. Ngo**

3:10 CHED **84.** Chemistry in the context of social justice. **M.M. Kirchhoff**

3:30 Panel Discussion.

Section E

San Francisco Marriott Marquis
Nob Hill A

Research in Chemistry Education

D. P. Cartrette, D. R. Mulford, *Organizers*

J. A. Schmidt-McCormack, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **85.** Comparative analysis of performance, post course performance, study time, motivation and perceived class quality in traditional, fully flipped, partially flipped and online chemistry 1A. **A. Holton**

1:55 CHED **86.** To flip or not to flip: The effectiveness of the flipped general chemistry class. **K.M. Hutchinson-Anderson**

2:15 CHED **87.** Academic Bottleneck: The impact of math skill on students' success in chemistry studies. **N. Glazer**, Y. Glazer

2:35 CHED **88.** Withdrawn.

2:55 Intermission.

3:10 CHED **89.** Clickers and cooperative learning as a combination to improve student learning in general chemistry as well as analytical chemistry courses. **D.J. Weiss**, R. Sandoval, M. Braseul, P. McGuire

3:30 CHED **90.** Evaluating the efficacy of modeling instruction in high school chemistry courses. E.M. Howard, **J.L. Jenkins**

3:50 CHED **91.** Effects of homework on learning: A classroom field experiment. **J.B. Nielson**, D. Nielson, B. Laney, K. Laney

4:10 CHED **92.** Memory and sensory cues: Does a sensory cue paired with chemistry content assist in later student achievement? **W.E. Schatzberg**

4:30 Concluding Remarks.

Section F

San Francisco Marriott Marquis
Nob Hill B

NMR Spectroscopy in the Undergraduate Curriculum

Financially supported by Bruker; ThermoFisher Scientific; JEOL; Anasazi Instruments

L. J. Anna, D. P. Soulsby, A. S. Wallner, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **93.** Integration of NMR spectroscopy into undergraduate research: HNMR analysis of ionic liquid monomers used in free-radical polymerizations. **B. McFarland**, M. Sea

1:55 CHED **94.** Undergraduate project for organic lab designed to teach multi-nuclear analysis by NMR. **S.M. Schelble**, J.M. Cook

2:15 CHED **95.** Utilizing NMR experiments to correctly assign closely spaced singlets in NMR spectra: A method to introduce 2D NMR spectroscopy in general organic chemistry laboratory courses. **A.M. Balija**, **D.D. Clarke**

2:35 Intermission.

2:50 CHED **96.** Multi-Outcome experiment development for organic chemistry utilizing NMR spectroscopy. **K. Yearty**, C.E. Glessner, R.K. Maynard, R.W. Morrison

3:10 CHED **97.** One-pot microwave experiments with NMR characterization of synthetic triazole esters. **A.M. Schoffstall**, B. Mayer, C.R. Butler, S. Robertson, K.A. Stewart, R.K. Shoemaker

3:30 CHED **98.** Incorporation of NMR spectroscopy in the introductory organic chemistry laboratory course as an effective means for promoting student active learning. **J.A. Cramer**

3:50 CHED **99.** Distinguishing aromatic and alkene NMR signals using specifically deuterated chalcones. C.A. Gehman, **C. Hamann**

4:10 Concluding Remarks.

Section G

San Francisco Marriott Marquis
Nob Hill C

Undergraduate Research Papers

Cosponsored by SOCED

J. V. Ruppel, N. L. Snyder, *Organizers*

C. V. Gauthier, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **100.** Synthesis of giant rhodium-based molecular gyroscopes as potential candidates for study of homeomorphic isomerization. **Z. Patton**

1:45 CHED **101.** PNP pincer ligand complexes of vanadium and zinc. **N. Onishi**, D. Unruh, M. Findlater, C.D. Abernethy

1:55 CHED **102.** Oxidation of methanesulfinate to methanesulfonate in the presence of catalase and superoxide dismutase. **N.M. Reed**, D.K. Wicht

2:05 CHED **103.** Novel cationic antimony containing compounds and their catalytic reactivity in organic reactions. **N. Pati**, M. Yang, M. Hirai, F.P. Gabbai

2:15 Intermission.

2:30 CHED **104.** Synthesis, characterization, and decomposition studies of a ruthenium N-heterocyclic carbene complex for transfer hydrogenation catalysis. J.R. Miecznikowski, **M.E. Morgan**, S. Bonitatibus, N.A. Bernier, C.A. VanAkin, B.Q. Mercado, R.H. Crabtree

2:40 CHED **105.** Aerogel films on indium tin oxide for electrochemical glucose biosensing. **N. Kosciuszek**, C. Brady, L. Sheard, A.S. Harper-Leatherman, M.C. Leopold

2:50 CHED **106.** Europium(III) tetracycline derivative species as potential bioprobe. **A. Riives**, G. Muller

3:00 CHED **107.** Probing chiral nanoparticle and protein interaction with isothermal titration calorimetry and molecular dynamics simulations. **H. Calcaterra**, W. Feng, Z. Qu, N. Kotov

3:10 Intermission.

3:25 CHED **108.** Deposition and characterization of thin carbon films. **A.P. Olson**, M. Berens, A. Heide, B.J. Winters

3:35 CHED **109.** Development of an organic-polyoxometalate-based framework utilizing a trigonally symmetric ligand. **K.S. Pearson**, **W.A. Neiwert**

3:45 CHED **110.** Post-synthetic Scholl oxidation for accessing large polycyclic aromatic hydrocarbons as structural component in metal-organic frameworks. **R. Ly**, Z.L. Magnuson, K. Sanchez, G. Pour, F. Uribe-Romo

3:55 CHED **111.** Alteration of membrane compositional asymmetry by $LiCoO_2$ nanosheets. M. Dogangun, M.N. Hang, J. Troiano, A.C. McGeachy, E. Melby, **J. Machesky**, J.A. Pedersen, R.J. Hamers, F. Geiger

4:05 Intermission.

4:20 CHED **112.** Porous PMMA-titania composites: Inverting the fabrication process to improve activity and durability. **J.D. Glover**, A.G. Horne, J.E. Boyd

4:30 CHED **113.** Analysis of Perovskite and its degradation mechanisms in ambient conditions. **P. De Peralta**, C. Kralik, M.V. Lee, K. Esparza

4:40 CHED **114.** Facile preparation of nanocrystalline tin oxide and photocatalytic dye degradation studies. **D. Mathew**, A.N. Venkatesha, R. Balan

4:50 CHED **115.** Bipyridine-functionalized BODIPY dyes for sensitizing near-infrared emission of lanthanide ions. **J.D. Bosonetta**, P.P. Senevirathne, H. He

5:00 Concluding Remarks.

Section H

San Francisco Marriott Marquis
Nob Hill D

Celebrating Chemistry through Outreach: Honoring the Legacy of Christine Jaworek-Lopes

I. J. Levy, D. K. Wicht, *Organizers*

B. E. Rios McKee, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **116.** Inspiring future chemists through green chemistry outreach. K. Anderson, M. Enright, **A. McCarthy**

1:55 CHED **117.** Recipe for success: How outreach has impacted Gordon College's ACS student chapter. **V. Curfman**

2:15 CHED **118.** GGC game changing beyond the classroom. **R.K. Kalman**, **G.E. Rudd**

2:35 CHED **119.** Infrared imaging devices light the way to new public outreach possibilities. **C. Barrett**, R.S. Black

2:55 Intermission.

3:10 CHED **120.** Hands, touchin' hands, reachin' out, touchin' me, touchin' you. **M.Z. Hoffman**

3:30 CHED **121.** Paying it forward—fun ways to engage the public in chemistry. **T. Halmi**, **G.L. Heard**, **L. Hogue**

3:50 CHED **122.** Students as change agents: GOLum (Green Organic Literacy Forum) outreach in the organic chemistry course. **I.J. Levy**

4:10 CHED **123.** Public engagement and science literacy. **B.Z. Shakhashiri**

4:30 Concluding Remarks.

Blending Chemistry & Culture: Undergraduate Research Abroad through ACS IREU Program

Sponsored by IAC, Cosponsored by CHED

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

‡ *Cooperative Cosponsorship*

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Sponsored by WCC, Cosponsored by CHED, CMA and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Textbooks & the Practice of Science: Before, During & After Gutenberg

Sponsored by CINF, Cosponsored by CHED and HIST‡

Withycombe-Charalambous Graduate Student Symposium

Sponsored by AGFD, Cosponsored by CHED

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Physical & Chemical Processes

Sponsored by ENVR, Cosponsored by CHED

Incorporating Polymer Science into the Classroom

High School & Community College

Sponsored by POLY, Cosponsored by CHED, MPPG‡ and PMSE

SUNDAY EVENING

Section A

Moscone Center
Hall D

General Posters

T. A. Miller, *Organizer*

7:00 - 9:00

CHED **124.** Teaching basic chemistry with MOOCS platform: An example of active learning. **Z. Own**

CHED **125.** Steps to change a large lecture class to an active learning class. **E.P. Kippenhan**

CHED **126.** Transforming the undergraduate chemistry experience through active learning: Evaluating pedagogical reforms within general and organic chemistry. **K. McCance**, E.D. Niemeyer

CHED **127.** Using a guided inquiry and experimental approach to teaching vibrational-rotational spectroscopy. **T.L. Longin**

CHED **128.** Assessing the effects of guided inquiry lab experiments on student learning quantum mechanics. **A. Mansfield**, S. Meyer, A.W. Jarnot, K.H. Bennett, C.J. Stromberg

CHED **129.** Accelerating organic synthesis and purification in the undergraduate organic chemistry lab–Fischer esterification. **J.E. Silver**, R. Klopper, O. Mneimne, F. Nancy, L.M. Esther, R.L. Lewis

CHED **130.** Microwave-assisted iodolactonization: A discovery-based green chemistry laboratory experiment. **C. Wang**, Y. Lin

CHED **131.** Surface tension, viscosities and refractive index of binary liquid systems. **H. Bascal**

CHED **132.** Investigating surface areas of nanoscale materials through a simple laboratory experiment. **D.S. Heroux**

CHED **133.** Measuring the thermal properties of polymers made from lactide and glycolide: An undergraduate chemistry experiment using differential scanning calorimetry. **B.K. Mohney**, **P.S. Corbin**

CHED **134.** Tale of two metabolites: Using the separation of urea and cholesterol to bridge the gap between general and organic chemistry. **N. Edwards**, F. Yepez Castillo

CHED **135.** Thienyl phosphine palladium (II) complexes: An introduction to hybrid materials in undergraduate laboratories. **B. Boardman**

CHED **136.** Substitution of organic solids with low toxicity compounds for binary phase diagrams in the undergraduate physical chemistry laboratory. **B.E. Dalesandro**, S.E. Hayik

CHED **137.** Expanding student access to instrumentation through the incorporation of portable infrared spectroscopy into the curriculum. **S. Meyer**, A. Mansfield, K.H. Bennett, C.J. Stromberg

CHED **138.** Biochemistry scavenger hunt. **S.E. Evans**

CHED **139.** 3D printable resources for chemical educators: Supporting laboratory learning activities via user-friendly devices. **L.A. Porter**

CHED **140.** Eliciting conceptual understanding via chemistry outreach: The development and implementation of a novel data collection method. **J.M. Pratt**, E.J. Yezierski

CHED **141.** Themed demonstration shows to increase community involvement. **B.J. Bellott**

CHED **142.** Chemical communication through infographics. **D. Diatta**, **S. Le**, **T. Le**, R. Singiser

CHED **143.** Infographics: Complex chemistry made simple. **M. Delgadillo**, **Y. Khan**, **K. Nguyen**, J.J. Meyers

CHED **144.** Science & culture: Engaging students with a local zoological park. **P.J. Carlson**, R. Bishop, L. Robinson, D. O'Gwynn

CHED **145.** Promise of palladium and the triumph of rhodium: Framing chemical research for public consumption through art. **D.B. Cordes**

CHED **146.** Maximizing potential: Building a bridge to success in the STEM field for the children of immigrant families through mentoring. **R. Romero**

CHED **147.** Advanced Authentic Research (AAR) program: A public school district research program. **J.V. Choe**

CHED **148.** Effects of introducing dye sensitized solar cells for renewable energy research to middle school students. **M.L. Grimminger**

CHED **149.** CSI dognapping workshop: A Sandia outreach program. **J.M. Sears**, T.J. Boyle, B.A. Hernandez-Sanchez

CHED **150.** Recruiting and supporting potential STEM teachers for southwestern Illinois. **S.D. Wiediger**, J.S. Krim, K. Barry, S.M. Locke, L. Cummings, T. Voepel

CHED **151.** Students' understandings of atomic orbital representations for carbon. **Z. Allred**, S. Bretz

CHED **152.** Modular 3D printed secondary structures for protein modeling. **P. Woodruff**

CHED **153.** Enthalpy and entropy changes in dissolving and precipitation reactions: Students' macroscopic observations and explanations. **T.N. Abell**, S. Bretz

CHED **154.** Students' use of symbolic and particulate representations to characterize bonding. **G.H. Allen**, C.J. Luxford, S. Bretz

CHED **155.** Cartoon character representations for the chemical structures of vitamins and other biologically significant molecules. **R.J. Schroeder**

CHED **156.** Chemisthenics: A literal VSEPR exercise. **C. Rezsnyak**

CHED **157.** Comparison of adaptive and traditional online homework systems in a preparatory chemistry course. **K.A. Kaiser**

CHED **158.** Development of online pre-laboratory activities in organic chemistry to improve students' preparation for laboratory. **J. Chaytor**, M. Al Mughalaq, H. Butler

CHED **159.** Tweet, for science!: A social media course for scientists at Caltech tackling inreach and outreach online. **O. Wilkins**, M.E. Davis, S. Mojarad

CHED **160.** Transitioning to eBooks: Student use of various textbook features. **E. Day**, N.J. Pienta

CHED **161.** Real-life examples as applied to general chemistry. **A. Burns**

CHED **162.** Trying on teaching: Being a learning assistant at a two-year college. **C.P. Schick**, K. Stennette, A. Palmer

CHED **163.** From failure to success in general chemistry: Learning strategies to the rescue. **E. Cook**, S.E. McGuire

CHED **164.** Teaching for success in solving organic synthesis problems. **N. Bode**, A.B. Flynn

CHED **165.** Flip your general chemistry class the easy way. **J. Moore**, M.A. Rau, L. Oxtoby, K. Kennedy

CHED **166.** Withdrawn.

CHED **167.** Incorporating new technologies into the chemistry curriculum at Elmira College. **C.E. Stilts**

CHED **168.** Teaching from this side of the fence: The benefits experienced by chemistry undergraduate teaching assistants. **S.B. Philipp**, C.V. Rich, T.R. Tretter

CHED **169.** Using screencasts to supplement classroom instruction. **D.B. King**

CHED **170.** Bridging chemistry. **R.R. Srinivasan**, **T. Nicholas**, **M. Rowane**, **L. Robinson**, **R. Juarez**, **D. Meyer**

CHED **171.** XUPharmPrep: A summer bridge program for first-year chemistry-prepharmacy majors. **M.R. Adams**

CHED **172.** Expansion of the science resource center into a STEM resource center. **S. Richards**, P.J. Iles, L.D. Giddings, R. Holcomb, M. Alvarez, R.V. Valcarce, R. Mcfarland, N.R. Bastian

CHED **173.** Does a better chemistry pre-test score mean a better grade in organic chemistry? **J.A. Jenson**

CHED **174.** Characterizing the alignment between inorganic chemistry faculty's learning goals and assessments. **J.H. Torres King**, E.J. Yezierski

CHED **175.** Organic chemistry students' understandings of molecular stability and reactivity in the context of substitution reactions. **M. Popova**, S. Bretz

CHED **176.** Associations between faculty beliefs about learning and instructional practice: Results from a national survey of postsecondary chemistry faculty. **R. Gibbons**, S. Villafane-Garcia, E. Laga, M.N. Stains, K.L. Murphy, J.R. Raker

CHED **177.** Investigation of absolute and relative scaling conceptions in an anatomy and physiology course. **J.M. Trate**, V. Fisher, A. Blecking, P. Geissinger, K.L. Murphy

CHED **178.** Exploring the roles of gender and prior knowledge on general chemistry students' cognitive structures. S. McLane, A. Milkey, M. Seibel, B. Kung, **O. Gulacar**

CHED **179.** Investigating and supporting students' understanding of the physical basis of interactions. A. Dragon, J. Pagdanganan, J.A. Loertscher, **V.M. Thorsell**

CHED **180.** Factors influencing the persistence and performance of chemistry majors. **B. Brando**, A.M. Baranger, A. Stacy

CHED **181.** Developing domain-specific reasoning and problem solving skills in organic chemistry. **M.R. Helix**, A.M. Baranger

CHED **182.** Withdrawn.

CHED **183.** Upgrading the role of teaching assistant in science teacher education: In-field teaching exercise in groups of students with different levels of competence. **G. Hornung**

CHED **184.** Using discovery, discussion, lab model at the elementary level. **K.M. Hutchinson-Anderson**

CHED **185.** Response and non-response rates in national surveys of postsecondary chemistry faculty: Implications for data analysis. **S. Srinivasan**, K.L. Murphy, J.R. Raker

CHED **186.** Developing a small batch approach to ACS Examination norms: A case study in inorganic chemistry. **K.A. Marek**, K.L. Murphy, J.R. Raker, J.J. Reed

CHED **187.** Report on the four-year old, science-developed, science-education minor at UCLA. **A.A. Russell**, J.W. Pang

CHED **188.** Investigating retention of concepts between the first and second semesters of organic chemistry. **W. Hollis**, W.E. Brenzovich

CHED **189.** Measures of success for an alternative starting point for at-risk STEM majors. **B.A. Davis**, J.K. Vohs, **M.A. Fisher**

CHED **190.** Math preparation for a GOB course as a predictor of success. **W.J. Donovan**

CHED **191.** Advancing graduate education in the chemical sciences with a modularazed curriculum. **C.V. Rice**, M.T. Ashby, M. Maher, R. Halterman

CHED **192.** NSF Graduate Research Fellowship Program for chemistry and chemical engineering students. **T.B. Higgins**, T.D. Kim, D. Rickey

CHED **193.** National Science Foundation programs that support chemistry education. **D. Rickey**, T.B. Higgins, T.D. Kim

CHED **194.** Impact of undergraduate research internships at Lawrence Berkeley National Laboratory. **L.E. Cote**, A.M. Baranger, E.M. Stone, M. Helix, C. Flood

CHED **195.** Research intensive honors program in chemistry. **T.S. Sempertegui Plaza**, **J.E. Haky**, D. Chamely Wiik, M. Cudic, M.C. Rodriguez

CHED **196.** Impacts of CUREs in chemistry and biology courses at three regional institutions. **E.M. Bowers**, J. Tomasik, D.J. Lecaptain, A. Mueller, K. Cissell, D.S. Karpovich, A.L. Martin, A.J. Ross, T. Sivy, J. Gittins, B.S. Harkness, K. Nitz, J. VanHouten

CHED **197.** *Drosophila melanogaster* food choice and survival on different sugars and sugar derivatives: An unorthodox learning experience for students not majoring in chemistry. **B. Budy**, J. Minbiole, J.S. Rhoad, P. Khol, J. Ribakova

CHED **198.** Fostering a sustainable and active membership in the Puerto Rico Section. **A.G. Colon**, **O.J. Morales Martinez**, H.A. Ocasio Rodriguez, S. Chaparro-Ruiz, J. Feng Baez, M. Leon, B. Ramos, E. Ferrer Torres, J.I. Ramirez Domenech

CHED **199.** Cooking the books: An honors seminar on the chemistry of cooking. **S. Hubbard**

MONDAY MORNING

Section A

San Francisco Marriott Marquis

Salons 1/2

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Symposium in honor of Marcy H. Towns

Cosponsored by WCC

S. Bretz, *Organizer*

M. Cooper, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **200.** Characterization of STEM faculty's conceptions and use of writing in STEM classes. **A.C. Moon**, S.A. Finkenstaedt-Quinn, A. Ruggles Gere, G.V. Szymczak

8:55 CHED **201.** Undergraduate students' goals for their chemistry laboratory coursework. **B.K. Dekorver**, M.H. Towns

9:15 CHED **202.** Achievement emotions in undergraduate organic chemistry. **J.R. Raker**

9:35 CHED **203.** Examining students' reasoning with mathematical models in the context of chemical equilibrium. **N.M. Becker**

9:55 Intermission.

10:15 CHED **204.** I will go out having learned something: Reflections on student learning in physical chemistry. **R.S. Cole**

10:35 CHED **205.** Planting seeds that make a difference! **L.E. Slocum**

10:55 CHED **206.** Framing the case: The importance of theory in structuring case studies in chemistry. **D.J. Wink**, J.V. Choe, M.T. Dianovsky, S. Lucas, M. Snow, L. Schroeder, G. Clark

11:15 CHED **207.** Increasing the influence and impact of CER: Developing high school teachers as chemistry education researchers. **E.J. Yezierski**

Section B

San Francisco Marriott Marquis

Salons 3/4

ACS-CEI Award for Incorporating Sustainability into Chemistry Education

Cosponsored by CEI

S. O. Obare, *Organizer, Presiding*

K. Aubrecht, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **208.** Green chemistry commitment: Addressing sustainability from the molecular-level to institutional-scale. **I.J. Levy**

9:10 CHED **209.** Incorporation of novel education approaches, including on-line gaming tools and 3D printing, intro graduate and undergraduate courses focused on sustainable materials. **A. Orlov**

9:40 CHED **210.** Socio-scientific issues-based chemistry teaching for incorporating education for sustainable development and green chemistry into secondary chemistry classrooms. **I. Eilks**

10:10 Intermission.

10:20 CHED **211.** Withdrawn.

10:50 CHED **212.** Sustainability and green chemistry education: Innovative and contextualized experiences from the undergraduate and postgraduate courses at the Federal University of São Carlos, Brazil. **V. Zuin**

11:20 CHED **213.** Incorporation of green chemistry and sustainability into the chemistry curriculum at Illinois Wesleyan University and globally. **R.S. Mohan**

11:50 CHED **214.** International perspective on green chemistry and sustainability education. **G.M. Bodner**

12:25 Concluding Remarks.

Section C

San Francisco Marriott Marquis

Salon 5

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Cosponsored by CCA, LSAC, SOCED and YCC

E. J. Brush, E. S. Garcia Sega, S. Nellutla, *Organizers*

E. Sega, *Presiding*

8:30 Introductory Remarks.

8:40 CHED **215.** MOFs @ CCs: Community college outreach through crystallographic research. **D.R. Manke**

9:00 CHED **216.** Combining 3D printing and and a chemistry lab to get home-schooled high school students excited about college. **J.D. Mendez**

9:20 CHED **217.** Outreach is HIP. **E.A. Alemán**, **K. Stone**

9:40 CHED **218.** Service learning across programs: A model for communicating aerosol chemistry. **B. Hames**, **H. Weizman**

10:00 Intermission.

10:15 CHED **219.** Informal STEM education: Resources for outreach, engagement and broader impacts. **J.R. Bell**

10:35 CHED **220.** Unexpected outcomes: Development and evaluation of STEM programs that promote confidence and build friendships. **S.S. Grathoff**, M.R. Wilhelm

10:55 CHED **221.** Symposium workshop on the fundamentals of chemistry outreach education: I. Program design. **E.J. Brush**, **E. Sega**, **S. Nellutla**

Section D

San Francisco Marriott Marquis

Salon 6

Advances in e-Learning & Online Chemical Education

L. A. Morsch, P. Sorensen, *Organizers*

D. A. Canelas, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **222.** Marvin JS and Smartwork5: Tools for online chemistry education. **A.D. Costache**, E. Hoffmann, C. Pruis

8:55 CHED **223.** Assignment-based repeated retrieval for learning chemistry. **J. Hearn**, E.L. Brown

9:15 CHED **224.** Learn how using WebAssign, Google Classroom and maybe even a little slack can make teaching general chemistry better for both students and faculty. **A.T. Griffin**

9:35 CHED **225.** Chem101: Next-generation classroom engagement tools built for chemistry students. **J. Weinberg**

9:55 Intermission.

10:10 CHED **226.** Computer simulations to help students learn general chemistry topics. **J. Selco**

10:30 CHED **227.** Learning organic mechanisms through spaced assignments. **E.L. Brown**

10:50 CHED **228.** PubChem as an educational resource for chemical information literacy. **S. Kim**, E. Bolton, S.H. Bryant

11:10 CHED **229.** Mobile animation tool: An app for creating and sharing chemical particulate animations. **J. Winter**

11:30 Concluding Remarks.

Section E

San Francisco Marriott Marquis

Nob Hill A

Chemistry Education Research: Graduate Student Research Forum

J. Donnelly, M. Popova, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **230.** Implementation of next generation science standards in high schools: Exploratory study. **A. Pierce**, C.E. Brown

8:55 CHED **231.** Evaluation of the teacher-scholar program: An integrated peer-learning program in the UC Berkeley College of Chemistry. **S.M. Tischhauser**, S.E. Limfat, S. Dilip, P. Marsden, M.T. Robak, A.M. Baranger

9:15 CHED **232.** Structural equation model for level of inquiry in undergraduate laboratory experiences and beliefs about chemistry on intent to pursue a post-baccalaureate degree. **A.R. Lunsford**

9:35 CHED **233.** Affects of gender and sexual orientation on belonging uncertainty in general chemistry. **J.A. Kroll**, K.L. Plath

9:55 Intermission.

10:05 CHED **234.** IRT as a tool to improve student performance. **B. Ohlsen**, C.H. Atwood

10:25 CHED **235.** Targeting the general chemistry bottom quartile through homework-based metacognitive training. **B. Casselman**, C.H. Atwood

10:45 CHED **236.** Considering the relationship between structure, properties, and function: How students connect these ideas across their introductory chemistry and biology courses. **K.P. Kohn**, S. Underwood, M. Cooper

11:05 CHED **237.** Team members' perceptions of how communication relates to the success of an interdisciplinary grant collaboration: The ChANgE Chem project. **N. Millick**, M. Orgill, S. Barakat

11:25 CHED **238.** Evaluating the impact of a redesigned chemistry course sequence for undergraduate life science majors. **C. Schnoebelen**, C. Hrycyna, J.A. Chmielewski, G.M. Bodner

11:45 Discussion.

11:55 Concluding Remarks.

Section F

San Francisco Marriott Marquis

Nob Hill B

Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

R. K. Boggess, *Organizer*

C. A. Burkhardt, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **239.** NSF S-STEM at Union College: Multidimensional mentoring model for student SUCCESS. **J.D. Kehlbeck**, S. Amanuel, G. Bizer, P. Catravas, R. Cortez, S. Kirkton

8:55 CHED **240.** Successful S-STEM scholarship program for undergraduate students at varying stages of degree progress. **A. Kubatova**, R. Simmons, D. Pedersen

9:15 CHED **241.** Increasing student success through the CSU S-STEM program. **K. Mardis**

9:35 Intermission.

9:50 CHED **242.** Infinity scholars, an NSF funded project that includes interdisciplinary undergraduate research. **R.R. Klepper**

10:10 CHED **243.** Seminar series for guiding students' development and exploration of chemistry careers. **P. Tandler**, J.A. Lupica, M.J. Dunphy

10:30 CHED **244.** Fostering interdisciplinary and investigative thinking and learning for first and second year chemistry students. **K.S. Owens**, A. Murkowski, A.M. Johansen, H. Price

10:50 Intermission.

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

11:05 CHED **245.** Building community in (inorganic) chemistry: Ideas from IONiC. **B.A. Reisner**, C. Nataro, S.R. Smith, A.K. Bentley, H.J. Eppley, E.R. Jamieson, A.R. Johnson, J.L. Stewart, L.A. Watson, N. Williams

11:25 CHED **246.** Impact of the summer institutes on faculty teaching and student achievement. **M.J. Graham**, J. Frederick, S.A. Strobel

11:45 Concluding Remarks.

Section G

San Francisco Marriott Marquis

Nob Hill C

Undergraduate Research Papers

Cosponsored by SOCED

C. V. Gauthier, J. V. Ruppel, *Organizers*

N. L. Snyder, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **247.** Operationally simple approach to indole derivatives from 2-alkenylanilines utilizing an oxidation-transannulation-elimination sequence. **J. King**, C.J. Monceaux

8:45 CHED **248.** Decarboxylation of amino acids via organocatalysis with various catalysts: A mechanistic study. **S. Deimling**, **H. Schriever**, D. Jackson, R.W. Morrison

8:55 CHED **249.** Rapid synthesis of N-(4-chlorobenzyl)morpholine. **J. Torgunrud**, L.I. Bobyleva, M.M. Bobylev

9:05 CHED **250.** Pyrazine nucleic acids: From small molecules to proto-informational polymers. **S.B. Wong**, **M. Gately**, E. Young, R. Krishnamurthy, A.L. Weber, T. Campbell

9:15 Intermission.

9:30 CHED **251.** Synthesis of multivalent glycooligomers for studying carbohydrate-protein binding. **N. Fendler**, **S.K. Eisenach**, N.L. Snyder

9:40 CHED **252.** Synthesis of hyaluronic acid-based phototherapeutic conjugates for diagnostic and therapeutic applications. **E. Xu**, K.E. Gonazlez, D. Dennis, J.V. Ruppel, N.L. Snyder

9:50 CHED **253.** Synthesis and characterization of RGD-conjugated alginate microparticles containing amphotericin B for the treatment of candida infections. **L.M. Aponte-Reyes**, L.M. Aponte-Cruz, M.P. Alvarez

10:00 CHED **254.** Synthesizing small lysyl oxidase inhibitors with β-aminoproprionitrile. **M.L. Williams**

10:10 Intermission.

10:25 CHED **255.** Synthesis of starch-functionalized dibromomaleimide for peptide delivery. **P.D. Wickremasinghe**, F.J. Hidalgo, O. Martini, P.M. Iovine, J.G. Schellinger

10:35 CHED **256.** Synthesis of a new series of alpha-(N)-heterocyclic thiosemicarbazone ligands and their Cu^{2+} metal complexes: Biological activity against human topoisomerase IIα and breast cancer cells. **V. Rand**, L.C. Ngo, X. Jiang, E.C. Lisic

10:45 CHED **257.** Independent measurements of lipids in mixed cell populations. **K. Estrada**, A.K. Stoeckman, N.E. Wolins

10:55 CHED **258.** Structural and functional characterization of arrythmogenic Q136P calmodulin mutant. **T. Bader**, S. Nelson, G. Veglia

11:05 Intermission.

11:20 CHED **259.** Synthesis and quantification of the chemical markers of melanin in complex biological matrices. **C. Weddle**, K.D. Sienerth, K. Glass

11:30 CHED **260.** Analyzing Sr isotopic ratios in surface and well water sources in northern Ohio. **A.F. Bauer**, A.R. Roerdink

11:40 CHED **261.** Comparison of nutrient and mercury contamination levels of surface water in lakes in Georgia and Maine using HACH and YSI surface water kits. **K. Hachat**

11:50 CHED **262.** Pottery residue analysis and archaeological application. **F.V. Macdonald**, K.L. Braun, C. Harper

12:00 Concluding Remarks.

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Textbooks & the Practice of Science: Before, During & After Gutenberg

Sponsored by CINF, Cosponsored by CHED and HIST‡

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Physical & Chemical Processes

Sponsored by ENVR, Cosponsored by CHED

MONDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Salons 1/2

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Symposium in honor of Marcy H. Towns

Cosponsored by WCC

S. Bretz, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **263.** Being in the right place, at the right time. **G.M. Bodner**

1:55 CHED **264.** Learning organic reaction mechanisms in a patterns of mechanisms curriculum. **A.B. Flynn**, K.R. Galloway, R.E. Featherstone, C. Stoyanovich, D. Webber

2:15 CHED **265.** Characterizing the development of mechanistic reasoning. **M. Cooper**

2:35 Intermission.

2:45 CHED **266.** Improving student success in general chemistry: Implementing a drop-back course. **N.J. Pienta**, M.B. Larkins, N.H. Johnson, A. Aspley, T.C. Barron

3:05 CHED **267.** Flavors of assessment in chemistry education and chemistry education research. **T. Holme**

3:25 CHED **268.** Meaningful learning and learning to mentor. **S. Bretz**

3:45 Intermission.

3:55 CHED **269. Award Address** (ACS Award for Achievement in Research for the Teaching & Learning of Chemistry sponsored by ACS Exams). From snowflakes to squid ink to guidelines for CER manuscripts: How chairlift rides, epicurean delights, and opportunities shape a career. **M.H. Towns**

Section B

San Francisco Marriott Marquis

Salons 3/4

Process Oriented Guided Inquiry Learning (POGIL)

R. S. Moog, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **270.** Introduction to POGIL and The POGIL Project. **R.S. Moog**

1:55 CHED **271.** POGIL as Gen.Ed.: Generating artifacts for the assessment of general education outcomes in the POGIL classroom. **J.G. Davis**

2:15 CHED **272.** Withdrawn.

2:35 Intermission.

2:45 CHED **273.** Implementing POGIL at a minority-serving institution. **T.D. Shepherd**

3:05 CHED **274.** Mirror images: Promoting students' assessment skills through reflection. **M.D. Perry**

3:25 CHED **275.** Improving process skills in a medium-sized organic chemistry lecture section at a minority serving institution. **K.R. Cousins**

3:45 Intermission.

3:55 CHED **276.** Development of professional skills via POGIL in an organic chemistry classroom. **D.A. Canelas**

4:15 CHED **277.** Development of a LEGO based POGIL activity for improving student's conceptual understanding of limiting reactants. **R.K. Campbell**, **I. Campbell**

4:35 CHED **278.** Representational competence: An examination of students' perceptions of chemical representations in POGIL activities. **T.D. Kim**, K. Miller

4:55 Panel Discussion.

Section C

San Francisco Marriott Marquis

Salon 5

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Cosponsored by CCA, LSAC, SOCED and YCC

E. J. Brush, E. S. Garcia Sega, S. Nellutla, *Organizers*

S. Nellutla, *Presiding*

1:30 Introductory Remarks.

1:40 CHED **279.** Chemistry day: Exploring, learning, and mentoring. **M. Rustagi**

2:00 CHED **280.** STEM after school: Undergraduate-led workshops for STEM outreach. **A.L. Smalley**

2:20 CHED **281.** Approximation to cultural heritage through chemistry as a way to promote interest in science and technology: The experience of the *Programa CHAT* in Peru. P. Gonzales, **B.C. Galarreta**, J. Nakamatsu, L. Ortega-San-Martín, I. Landa Fitzgerald, S. Córdova

2:40 CHED **282.** Exploring matter: An interactive, inexpensive chemistry exhibit for museums. **S.L. Murov**

3:00 CHED **283.** Outreach as an essential element of research training: Exposing REU participants to the divide in STEM-field enthusiasm. **K.C. Tvrdy**, A. Schoffstall, S.B. Braun-Sand, C. Rolsma

3:20 Intermission.

3:35 CHED **284.** Juice from juice: Bringing solar energy education to the classroom. **M. DeBoever**, J.D. Schuttlefield Christus

3:55 CHED **285.** Discovering inexpensive, effective catalysts for solar energy conversion through educational outreach. **J.D. Schuttlefield Christus**, M. DeBoever

4:15 CHED **286.** Chemistry open lab night as professional development for middle school and high school educators. **E.J. Brush**, **C.D. King**

4:35 CHED **287.** Connecting Maine high school students with USM STEM undergraduates through a chemistry lab experience. **L. Benedict**, C.M. Prudente, M. Hausman

4:55 CHED **288.** Impact of science nights: Incorporation of a hands-on science outreach/service-learning project into a freshman-level college chemistry course. **F.M. Yarberry**

5:15 Discussion.

Section D

San Francisco Marriott Marquis

Salon 6

Advances in e-Learning & Online Chemical Education

D. A. Canelas, P. Sorensen, *Organizers*

L. A. Morsch, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **289.** Design-based research to improve student perceptions of autonomy and efficiency in an online learning system. **R. Sansom**, R. Bodily

1:55 CHED **290.** Analysis of cognitive science design features and student use of online learning systems for general chemistry. **E.E. Wilson**, S. Kennedy

2:15 CHED **291.** Implementation of spectroscopy software, technique videos, and a lab practical in the first semester of the organic chemistry laboratory. **M.T. Wentzel**

2:35 CHED **292.** Chemistry Class Advantage™: Teaching the relevance of organic chemistry. **A.R. Dick**, R. Schenck, K.C. Schwall, S.E. Miller

2:55 Intermission.

3:15 CHED **293.** Building and assessing the Libretexts Project (nee ChemWiki). **D.S. Larsen**

3:35 CHED **294.** Innovative e-learning curricula, resources, methods and data applications were developed as foundations for building a chemistry centered Science, Technology, Engineering, (Arts), Mathematics, STE(A)M, learning model using a non-science majors chemistry course and engineering/computer science courses as exemplars. **R.J. Rusay**, B. Koo, D.S. Larsen, G. Dasgupta, R. Dougherty

3:55 CHED **295.** Interinstitutional chemistry communication practice: The ins and outs of implementing an international collaboration. **L.A. Morsch**, **B. McCollum**

4:15 CHED **296.** Interinstitutional chemistry communication practice: Technological, social, and disciplinary barriers. **B. McCollum**, **L.A. Morsch**

4:35 Concluding Remarks.

Section E

San Francisco Marriott Marquis
Nob Hill A

International & Multicultural Perspective

Cosponsored by IAC

S. J. Hansen, W. E. Schatzberg, *Organizers*

C. T. Cox, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **297.** Cultural diversity and its effects on what is happening in chemistry classroom. A study on Malaysian multi-cultural context. **M. Karpudewan**

1:55 CHED **298.** One country, two cultures: A multi-perspective view on Israeli chemistry teachers' beliefs about teaching and learning. **M. Hugerat**

2:15 CHED **299.** Use of in-class, interactive strategies to promote attention, interest, and generation of explanations in a large enrollment chemistry course at the University of Costa Rica. **B. Fernadez-Solano**, **E. Jimenez Alvarado**, **S. Sandi-Urena**

2:35 CHED **300.** Teaching multi-scale modelling to physicists and chemists in a unique class: Project-based learning in master's degree in the context of a French university. **F. Jolibois**

2:55 Intermission.

3:10 CHED **301.** Approaches to improve chemistry education: Two case studies in Costa Rica. **S. Sandi-Urena**

3:30 CHED **302.** Student perception of multiple-choice general chemistry exams and its influence in the teaching-learning process at the University of Costa Rica. **E.N. Jimenez-Alvarado**

3:50 CHED **303.** DivCHED IAC's collaborative outreach to delegates of the Cuban Chemical Society. **R.M. Kelly**, C.H. Atwood

4:10 CHED **304.** Picking up the fork in the road. **S.J. Hansen**

4:30 CHED **305.** European Science Education Research Association Conference 2015: What did I learn and how did it change my research. **W.E. Schatzberg**

4:50 Concluding Remarks.

Section F

San Francisco Marriott Marquis
Nob Hill B

Curricular Innovations in Undergraduate Chemical Education Impacted by NSF

C. A. Burkhardt, *Organizer*

R. K. Boggess, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **306.** National Science Foundation programs that support undergraduate chemistry education. **T.D. Kim**, T.B. Higgins, D. Rickey

1:55 Discussion.

2:15 Intermission.

2:30 CHED **307.** Curriculum innovation through collaborative introduction of MALDI-TOF mass spectrometry, undergraduate research methodologies, and POGIL instructional methods. **C. Lutz**, **J. Grant**, P. Pieper, A. Aspaas

2:50 CHED **308.** Using threshold concepts to drive curriculum reform in biochemistry. **J.A. Loertscher**, J.E. Lewis, V.M. Thorsell

3:10 CHED **309.** Structure and evaluation of a flipped general chemistry course as a model for both small and large gateway science course at an urban public institution. **D.M. McGregor**, M. Deri, P. Mills

3:30 Intermission.

3:45 CHED **310.** Relating chemistry to healthcare and MORE (NSF DUE 1431926). **G. Clark**

4:05 CHED **311.** Undergraduate crystallographic education made possible by the NSF Major Research Instrumentation Program. **J. Tanski**

4:25 CHED **312.** Building the beast-developing and assessing effective cyberlearning within the libretexts open access textbook resource. **D.S. Larsen**

4:45 Concluding Remarks.

Section G

San Francisco Marriott Marquis
Nob Hill C

Undergraduate Research Papers

Cosponsored by SOCED

J. V. Ruppel, N. L. Snyder, *Organizers*

C. V. Gauthier, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **313.** Determination of aluminium background signal fraction in the Q_{weak} experiment. **J. Butler**

1:45 CHED **314.** Molecular plasmonics for ultralow-power, multicolor electrochromic devices. **G.J. Stec**, A. Lauchner, Y. Cui, P.J. Nordlander, N.J. Halas

1:55 CHED **315.** Fano-type resonances detected at catalytic surfaces with ATR-IR. **J. Lindale**, D.G. Kovacs

2:05 CHED **316.** Exploring the carbon chemistry of the galactic interstellar medium: Photochemical stability studies of polycyclic aromatic hydrocarbons by argon matrix isolation spectroscopy. **S. Erickson**, A. Mattioda, G. Cruz-Diaz

2:15 Intermission.

2:30 CHED **317.** Adsorption of water-soluble peptoids to silica monitored by second harmonic generation. **A. Calkins**, A.A. Fuller, G.Y. Stokes

2:40 CHED **318.** Doxorubicinone interactions with DNA: A spectroscopic comparison. **E.J. Curtis**, S. Glazier

2:50 CHED **319.** Sulfate esters in our atmosphere. **K.J. Angle**, A. Fuller, T.A. Humphry, E.A. Stone, Y. Chen

3:00 CHED **320.** Controlling electronics with chemistry: A computational study of molecular electronics. **J. Metzger**, B. Topham

3:10 Intermission.

3:25 CHED **321.** Reaction pathway analysis guided by conceptual density functional theory. **J.K. Niblo**, R.J. Olsen

3:35 CHED **322.** Thermodynamic models to aid the experimental design of multivalent systems: Polymer brushes and nanoparticles. **I. Kopyeva**, R. Kumar, J. Lahann

3:45 CHED **323.** Search of new anti-cancer compounds through combined QSAR and virtual screening of allosteric LSD1 inhibitors. **G.L. Luiz Genesi**, V.G. Maltarollo, F.d. Emery, G.H. Trossini

3:55 CHED **324.** Synthesizing phthalimide derivatives as dual kinase inhibitors targeting angiogenesis. **V.C. Miles**, M. Ismail, R. Komati, H. McFerrin, J. Sridhar

4:05 Intermission.

4:20 CHED **325.** Using 3D printing and magnets to model chemical reactions. **K. Smiar**

4:30 CHED **326.** Expanding the scope of single molecule FRET spectroscopy at primarily undergraduate institutions. **J. Howe**, **J. Flores**, G. Walters, K.M. Hamadani

4:40 CHED **327.** Investigating enzyme active-site geometry and stereospecificity in the undergraduate biochemistry lab. **S.R. Roschdi**, T.J. Gries

4:50 CHED **328.** Withdrawn.

5:00 Concluding Remarks.

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Agricultural & Food Chemistry

Cosponsored by AGFD‡ and SOCED‡

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **329.** Isolation, characterization, and identification of bacteria in yogurts and probiotics. **K. Negron-Teron**, M. Class, N.M. Soto, O. Ortiz, J.A. Cardé

CHED **330.** Survey of commercially available soy sauces for the presence of histamine, putrescine, and cadaverine. B.A. Clement, **R. Sanchez**, **S. Ponce**, M. Smith, T. Wiley

CHED **331.** Comparison of purple and yellow nutgrass tubers and sedge, *Cyperus rotundus* and *C. esculentus*, for antibiotic activity. B.A. Clement, **R. Sanchez**, S. Stanford, **S.D. Jenkins**, **S. Ponce**

CHED **332.** Analysis of kombucha tea fermented with blueberry juice. **B.T. Copet**, F. Mann

CHED **333.** Is it safe to vape? **P. Schwartz**, W. Meyers, B. Anderson, P. Moon, K. Cornell

CHED **334.** Solvent variations of the Briggs-Rauscher reaction. **C. Trost**, A. Figuereo, M. Roche, L. Albertini, L.C. Fernandez

CHED **335.** Quantification of catechin compostion in *Camellia sinensis:* Comparing different leaf processing methods. **L. Krings**, M. Ehlert, C. Hull, B. Klein, L. Lanum, D. Choffnes

CHED **336.** Characterization and quantification of volatiles over the fermentation process in beer using headspace solid-phase microextraction and gas chromatography/mass spectroscopy (HS-SPME-GC/MS). **Z. Huang**, L. Benedict

CHED **337.** Comparative analysis of antioxidant and anti-amyloidogenic properties of various polyphenol rich phytoceutical extracts. **K. Kleinrichert**, B. Alappat

CHED **338.** Powerful plants: Antioxidant capacity of selected plants. **C. Curiac**, J. Alvarodiaz, L. Bontemps, L. Castellar, J. Cerda, A. Figuereo, C. Trost, L.C. Fernandez

CHED **339.** Effects of metal salts and anoxia on the photodegradation of red food dyes in solution. **C. Boyles**, S.J. Sobeck

CHED **340.** Cocoa liquor provenance determination using trace elemental signatures. **P.E. Sudol**, L. Monroe, S. Maloney, R. Khalsa, R.E. Sours, S.E. Stitzel

CHED **341.** Filled hydrogels as delivery systems for control release of flavored nanoemulsions. **A. Kwan**, G. Davidov-Pardo

CHED **342.** Aquaponics and the effect on the cell wall. **J. O'Flanagan**, C. Esslinger, A. Marry

CHED **343.** Colorimetric detection of gentamicin in milk using functionalized gold nanoparticles. **J.C. Gukowsky**, C. Tan, L. He

CHED **344.** Analysis of heavy metals in livers and fillets of spotted seatrout (*Cynoscion nebulosus).* **P. Intravichit**, B. Adair

CHED **345.** Effect of common food preservatives, Butylatedhydroxytoluene (BHT) and sodium benzoate, on the survival rate and behavior of *Daphnia magna*. R. Valedon Arce, L. Narvaez Mejias, **M. Barriera Diaz**, J.I. Ramirez Domenech

CHED **346.** Method development for determination of capsaicinoids from complex food matrices. **J. Peschke**, S. Chakraborty

CHED **347.** Cafestol concentration comparison in coffee beans. **K. Houser**, E.A. Baldauff

CHED **348.** Determination of zinc by flame atomic absorption spectroscopy using chemical digestion for complex beer matrices. **C. Wentworth**, J. Bruce, R. Patnaude, L. Benedict, Z. Bodah

CHED **349.** Validation of short sequence repeats present in *Triticum monococcum*. **H. Wesselman**, S. Fox, A.L. Smalley

CHED **350.** Tracking calcium content throughout the craft brewing process via flame atomic absorption spectroscopy. **J. Bruce**, J. Balsamo, C. Wentworth, C. Mahaffey, N. Sanborn, L. Benedict

CHED **351.** Evaluation of Amazon products: Drying and lipids extraction of cupuassu (*Theobroma grandiflorum)* seeds. **M. Pereira**, P.K. Silva Silva, L.C. Guedes Coelho Marinho, M.R. Carvalho Morais, W. da Luz Rodrigues

Section I

Moscone Center
Hall D

Undergraduate Research Posters

‡ *Cooperative Cosponsorship*

Analytical Chemistry

Cosponsored by ANYL and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **352.** Identification of volatile organic compounds present in cigarette smoke via purge-n-trap coupled with GC/MS. **P. Skersick**, C.H. Lisse

CHED **353.** Quantitative identification of volatile organic compounds and free base nicotine present in electronic-cigarette vapor via GC/MS detection. **E. Smith**, C.H. Lisse

CHED **354.** Self-assembly of monolayers on graphene with pyrene and cyclodextrin derivatives. **E. Swanson**, X. Zhen, P. Buhlmann

CHED **355.** Analysis of e-cigarette fluid with Direct Sample Injection (DSI) GC-MS/MS. **K. Rogers**, K. Bisceglia, L. Huang

CHED **356.** Quantification of B-vitamins in multivitamin dietary supplements though HPLC-MS. **T. Vu**, S. Pribil, K.J. Sorauf

CHED **357.** Withdrawn.

CHED **358.** Comparison of Oasis WCX and Oasis HLB sorbents for polar organic chemical integrative samplers and for solid phase extraction of wastewater for detection and quantification of amphetamine-type stimulants. **M. Fulmer**, A. Loftis, J. Donegan, T.H. Boles

CHED **359.** Withdrawn.

CHED **360.** Withdrawn.

CHED **361.** Investigation into the effect of aging and grain content on the chemical composition of whiskey. **W. Pugh**, R. Lahti

CHED **362.** Comparison of Bisphenol A concentrations in Zebrafish tissue and the surrounding water using UPLC-MS/MS. **E. Dornisch**, S. Ramakrishnan, M. Gessel

CHED **363.** The isolation and determination of two related compounds from the leaf gel of *aloe cameronii*. **A. Theberge**, A. Trowbridge, R.L. Bretz

CHED **364.** Characterizing dissolved organic material in local lakes and streams through excitation-emission fluorescence spectroscopy and parallel factor analysis. **S. Pribil**, T. Vu, K. Sorauf

CHED **365.** Chemically-induced droplet coalescence in a droplet microfluidic device. **D.G. Horvath**, D. Pluhar, P. Abbyad

CHED **366.** Using SPME-GC/MS to identify attractive odorants in the bacterial food sources of *C. elegans*. **S. Worthy**, G. Rojas, E. Glater, C.J. Taylor

CHED **367.** Covalent modification of multiwall carbon nanotubes with β-cyclodextrin for enhanced electrochemical detection of uric acid. **S. Gillespie**, M.A. Schwarzmann, A. Kane, C. Bowles, M. Trawick, M.B. Wayu, M.C. Leopold

CHED **368.** Neurochemical study of zebrafish using fast-scan cyclic voltammetry. **M. Furgurson**, M. Shin, M.A. Johnson

CHED **369.** Development of a facile method for the screening of prescription medications of abuse employing a portable GC/MS. **R. Shen**, S. Michalsky, D.C. Collins

CHED **370.** Eliminating backflash in gas chromatography through the use of zero-solvent-volume thermal desorption injectors. **S. Michalsky**, A. Tolzmann, S. Grover, D.C. Collins

CHED **371.** Development of layer-by-layer design of xerogel-based amperometric first generation biosensors on wire electrodes. **G.E. Conway**, M.C. Leopold

CHED **372.** Edible oil fingerprinting using direct infusion ESI-MS and principal component analysis. **M. McNamara**, L. Loukotkova, G. Gamboa da Costa

CHED **373.** Method development for the analysis of Bisphenol A (BPA) in milk. **A.M. Encerrado**, W. Lee

CHED **374.** Analysis of FAME and sterol content in biodiesels using PCA. **A. Clifford**, A.M. Hupp

CHED **375.** Analysis of raw materials in a veterinary topical analgesic. **A. Franzen**, E. Westemeier, J. Erickson, J.E. Larson

CHED **376.** Green chemistry analysis of metal complexes by MALDI-TOF. **C. Jernigan**, G.R. Dubay

CHED **377.** Comparative studies on the interactions of nanoceramics (metal oxides) with hemoglobin. **T. Batte**, E.E. Mojica

CHED **378.** Evaluation on the interaction of nanomaterials with enzymes (catalase and lipase) using optical spectroscopy. **K. Chhe**, E.E. Mojica

CHED **379.** Method development for analysis of illicit drugs/amphetamines in biological samples. **L. Reilly**, E.E. Mojica

CHED **380.** Discrimination of fluoroquinolone antibiotics using Raman spectroscopy. **A.E. Kuptsow**, E.E. Mojica

CHED **381.** Phenol content and its relationship to the antioxidant activities of different commercial tea samples. **A. Villaggi**, E.E. Mojica

CHED **382.** Quantification of quorum sensing components produced by bacterial biofilms. **K. Kougl**, J.A. Stenken

CHED **383.** Monitoring the water quality of selected Billion Oysters Project (BOP) restoration sites. **J. Zapata**, E. Jones, G. DiMeglio, R. Kline, L.B. Birney, E.E. Mojica

CHED **384.** Carboxylic acid multi-walled carbon nanotubes modified with β-cyclodextrin for the detection of uric acid on an electrochemical sensor. **M.A. Schwarzmann**, S.D. Gillespie, M.B. Wayu, L. Hughes, M.C. Leopold

CHED **385.** NMR studies with $^{1}J_{CC}$ coupling and computational modeling to identify preferred tautomers in austrocortinin. **G. Versfeld**, J.R. Powell, J.K. Harper

CHED **386.** First generation amperometric biosensor to detect galactosemia. **T. Munoz**, C. Steele, W. Case, M.C. Leopold

CHED **387.** Chemical and structural analysis of metronidazole and its derivatives. **S. Azimi**, D. Athanasopoulos, R.K. Upmacis

CHED **388.** Evaluation of novel massive projectiles for nanoscale secondary ion mass spectrometry. **A. Vinjamuri**, M. Eller, G.D. Shuffield, E.A. Schweikert

CHED **389.** Analysis of a series of dietary supplements via energy dispersive X-ray Fluorescence Spectroscopy (EDXRF). **W. Bair**, S. Maurice, E. Roberts-Kirchhoff, M.A. Benvenuto

CHED **390.** Analysis of a series of coins of the Byzantine Empire via energy dispersive X-ray Fluorescence Spectroscopy (EDXRF). **W. Bair**, J. Pothoof, G. Nguyen, M. Bhagwagar, M.A. Benvenuto

CHED **391.** Development of metal ion specific sol-gel targets for trace metal total reflection X-ray fluorescence analysis. **A. Butler**, A. Arndt, R.N. Dansby-Sparks

CHED **392.** GC-MS analysis of cyanuric acid in swimming pool waters. **D. Chun**, C. Lehr

CHED **393.** Determining extracellular sulfatase SULF1 concentration as a biomarker to detect the onset of breast cancer using an electrochemical approach. **A. Nguyen**, K. Vu, K. Gardiner, Z. Huang, Z. Wang

CHED **394.** Exploration of the upper mass limit of CRAFTI through protein cross-section analysis. **B. Pope**, D.V. Dearden

CHED **395.** Improving the technique of simultaneous chromatography and electrophoresis by employing vertical sealing margins to achieve a flat-continuous solvent flow profile. **R.E. Soto Alvarez**, J.D. St. Jeor, E. Naef, D.C. Collins

CHED **396.** Incorporating statistics to probe solvent mechanisms. **A. Lonski**, M.J. D'Souza

CHED **397.** Evaluating the relationship between chemical profiles and cryptic species of *Sarcophyton* soft corals in Palau using both supervised and unsupervised statistical learning. **E.M. Maloney**, **J. Chari**, R.T. Botts, T.S. Davis, O.A. Alvarado, B.J. Chicoine, C. Brayton, C.S. McFadden, K.N. Maloney

CHED **398.** Use of polynomial regression techniques to predict solvent mechanisms for benzoyl cyanide. **E. Brandenburg**, M.J. D'Souza

CHED **399.** Spectroscopic properties of hydroxycinnamic acids under acidic, neutral, and basic conditions. **J. Farshi**, E.E. Mojica

CHED **400.** Geochemical analyses at Eagle Cave, TX: X-ray diffraction and accelerator mass spectrometry radiocarbon dating. **J. DeYoung**, K.L. Steelman

CHED **401.** Raman spectroscopy and density functional theory calculations of phenolic acid derivatives. **S.J. Pace**, E.E. Mojica

CHED **402.** Evaluation of different methods in the extraction of active compounds from bee propolis. **L.O. Wyan**, E.E. Mojica

CHED **403.** Binding of oxytetracycline and doxycycline with nanoceramics. **H.N. Tonn**, H.B. Jufer, E.E. Mojica

CHED **404.** Analysis of sulfa drugs using Raman spectroscopy and Density Functional Theory (DFT) calculations. **A.R. Javornik**, E.E. Mojica

CHED **405.** Sample preparation and analysis of NSAIDs (Non-Steroidal Anti-Inflammatory Drugs) in environmental water samples. **E. Jones**, E.E. Mojica

CHED **406.** Building a low cost Raman spectrometer. **S. Thibado**, J.R. Williams

CHED **407.** Investigation of charcoal-based electrically conductive paint. **A. Arslanian**, W.E. Schatzberg

CHED **408.** Strengths and weaknesses of glass pH probes quantified: An advanced undergraduate chemistry laboratory. **A. Corral**, J.C. Goeltz

CHED **409.** Improving a method for detecting fish exposed to cyanide via thiocyante ion excretion using High Performance Liquid Chromatography (HPLC). **R.J. Metivier**, N.E. Breen, A. Rhyne

CHED **410.** Lead detection by hair analysis. **D.L. Sullivan**, D.J. Schauer

CHED **411.** Analyzing the binding relationship between curcuminoids and HSA by steady state fluorescence spectroscopy. **G.J. Myres**, O. Michels, M. Amman, M. Roozeboom

CHED **412.** Molecular dynamics simulation study of chiral recognition by dipeptide-based molecular micelles. **K. Krause**, J. Ingle, E. Billiot, F.H. Billiot, Y. Fang, K.F. Morris

CHED **413.** Isolation of possible antifungal compounds from *Aloe barbadensis*. **H. Hirata**, R.L. Bretz

CHED **414.** Analysis of wastewater samples for opioids using collection by passive and grab sampling and extraction by reversed-phase and mixed-mode sorbents. **W. Parker**, K. Moffitt, A. Loftis, T.H. Boles

CHED **415.** Identification and characterization of analyte binding sites in chiral molecular micelles. **J. Ingle**, K. Krause, E. Billiot, F.H. Billiot, Y. Fang, K.F. Morris

CHED **416.** Withdrawn.

CHED **417.** Structure relationship study comparing binding affinities of pyridine-2,6-dicarboxylic acid (DPA) with DPA derivatives to develop alternative small chelating molecules. **K. Page**, **M. Kirkland**, S.G. Tajc

CHED **418.** Fluorescent detection of hydrogen sulfide (H_2S). **M. Maher**, **D. Newman**, K. Peterson

CHED **419.** Spectrophotometric method for the determination of nitrite with a single reagent. D.A. Habboush, **R. Alahmadi**, **S. Alsenani**

CHED **420.** Performance enhancing supplements: Do we need stronger regulations? **K. Baran**

CHED **421.** Derivatization, DLLME, and GC-FID analysis of mercury in fish tissue. **A. Narro**, L.A. Curry

CHED **422.** Effect of pH on properties of amino acid based surfactants. **Z. Ramos**, C. Lewis, E. Billiot, F.H. Billiot, K.F. Morris

CHED **423.** Spectroelectrochemical analysis of trace metals in gunshot residue. **C.E. Ott**, J.N. Richardson

CHED **424.** Preparation of organo-silica monolithic columns for applications in capillary liquid chromatography using thiol-ene click reaction. **A. Burkus-Matesevac**, Z. Zajickova

CHED **425.** Theoretical analysis of the standard reduction potential for the irreversible redox process of methionine. **R. Krupa**, J. Roberts, L.A. Sombers

CHED **426.** Testing agreements between NMR and mass spectrometry HX method. **L. Downer**, M. Weerasinghe, D.D. Weis

CHED **427.** Using High Pressure Liquid Chromatography (HPLC) for the analysis of artificial sweeteners and caffeine in soft drinks, carbonated waters, and singles to go packets. **D. Martin**, R. Chinni

CHED **428.** Development of a paper-based analytical device for heparin. **C. Norris**, J.M. Esson

CHED **429.** GC-MS analysis of Chinese baijiu liquor flavored as American bourbon whiskey. **C. Nowlin**, R.L. Silvestri

CHED **430.** Production and analysis of aluminum fluoride phosphate glasses synthesized by a sol-gel method. **J. Fletcher**, C.B. Brennan, N. Marrero-Silva

CHED **431.** Fixed-time kinetic spectrophotometric determination of biotinylated aptamers. **B. Mandella**, D. Spikerman, A.G. Cavinato

CHED **432.** Degradation of tetracyclines in anaerobic digestion using solid phase extraction and HPLC. **C. Cruse**, E.D. Conte, A.J. Abdulrheem, C. Fullington

CHED **433.** Study of L-phenylalanine-based ionic liquids as stationary phases for GC. **K. Raut**, I. Kimaru

CHED **434.** Determination of the dissociation constants of triprotic acids with broadly ranging pK_as. **H. Do**, G.Z. Goloverda, V.L. Kolesnichenko

CHED **435.** Determination of BAC in varying hemoglobin levels. **K. Klein**, K. Opel

CHED **436.** Detection and quantification of amphetamine in buried rat brain, heart, and liver at different stages of decomposition. **C.R. Mendralla**, K. Scott, M. Drumm

CHED **437.** Optimizing cloud point extraction for stripping anodic voltammetry of transition metals. **C. Quartermaine**, M. Hawkins, C.A. Rusinek, A.F. Bange

CHED **438.** Withdrawn.

CHED **439.** Towards an arsenic-specific aptasensor based on AuNPs/thiol interactions. **K. Vega-Figueroa**, I. Mayorga, A. Rivera, E. Nicolau

CHED **440.** Analysis of catalytic isomerization and degradation of methyl-parathion by mixed metal oxide nano-fibers using LC-MS methods. M.M. Allard, C.C. Perry, **S. Merlos**

CHED **441.** Analysis of kinase substrate peptides by capillary electrophoresis. **S. Cook**, C.T. Culbertson

CHED **442.** Survey of the chemical and physical properties of deep eutectic solvents. **A. Beyer**, **J. Salazar**, M.E. Johll

CHED **443.** Spectroelectrochemical determination of lead and zinc through attenuated total internal reflectance stripping voltammetry. **R.J. Shaffer**, J.N. Richardson

CHED **444.** Analysis of fish oil supplements for omega-3 content and heavy metal contamination. **V. Stafford**, J.R. Williams

CHED **445.** Electrochemical properties of amines on planar platinum surfaces. **K. Wong**, M. Ma, E.C. Landis

CHED **446.** CO-extraction of lead and cadmium by cloud point extraction as a pre-concentration method for analysis by square wave stripping voltammetry. **M. Hawkins**, C. Quartermaine, A.F. Bange, C.A. Rusinek

CHED **447.** Design and development of sarcosine sensors utilizing nanomaterials. **E. Doll**, N. Labban, M. Pannell, H. Kerins, M.B. Wayu, J.A. Pollock, M.C. Leopold

CHED **448.** Extraction and analysis of agarita (*Mahonia trifoliolata)*. **M.A. Boyle**, N.A. Leed, B. Leverett, B. McBurnett

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

CHED **449.** Comparison of the caffeine content of popular brewing methods. **T.L. Self**, K. Cossey, C. Mills

CHED **450.** Determination of illicit drug metabolites in wastewater using GC-MS following a Dean-Stark extraction. **M. Wiernusz**, G.P. Foy

CHED **451.** Determination of cadmium in water samples by spectrophotometric methods. **T. Rutherford**, S. Hubbard

CHED **452.** Design of the time-of-flight mass spectrometer using chemically developed semi-conductive electrode as a multi-potential ion guide. **D.V. Kravchuk**, J. Nederhoff, M. Flesch, C. Hanson

CHED **453.** Minimizing diacetyl formation in beer by controlling fermentation parameters. **S.M. Brennan**, R.A. Hunter

CHED **454.** HPLC analysis of juglone in black walnut hull supplements. **A. Dixon**, Y. Liu

CHED **455.** Exploring Solid Phase Analytical Derivatization (SPAD) as a sample preparation method for quantitative analysis by GC-MS. **A. Bieber**, Y. Mei-Ratliff

CHED **456.** Determination of lead concentration in water samples using spectrophotometric and electrochemical methods. **A. Engelkes**, S. Hubbard

CHED **457.** Analysis of reducible species within natural dissolved organic matter using attenuated total reflection Fourier transform infrared spectroscopy. **D. Fleischmann**, D.R. Baluha

CHED **458.** Comparative study of heavy metal levels in various eye cosmetic products. **A. Lipniskis**, M.A. Fisher

CHED **459.** Applying chemistry to questions in neuroscience: HPLC-DAD/MS analysis of *Passiflora incarnata*. **K.A. Perrotta**, A. Weiss, S. Cameron, A. Halpern, T. Luck, P. Maehler, A.J. Stavros, C.M. Ingersoll, J.A. Teissere

CHED **460.** Aptamer selection assisted by graphene oxide. **J.K. Carter**, B. Mandella, D. Spikerman, A. Harris, G. Rodriguez, A.G. Cavinato

CHED **461.** Electrospinning of quantum dot-doped organic polymers for differential detection of targeted chemicals. **M. Lister**, D. Morris, M. Hicks, J. McNeal, D.E. Riegner

CHED **462.** Optimization of sarcosine oxidase isolation and purification for use in amperometric biosensors. **N. Labban**, E. Doll, **H. Kerins**, M. Pannell, W. Mulugeta, J.A. Pollock, M.C. Leopold

CHED **463.** Investigation of biodiesel-diesel blends using GCMS and PCA. **C. Brown**, R. Dean, A.M. Hupp

CHED **464.** Analysis of petroleum products in lakes of the Wasatch watershed, Salt Lake City, Utah. R.M. Hyde, **L. Miller**

CHED **465.** Enhanced reproducibility for the analysis of polycyclic aromatic hydrocarbons in river water. **D. Herrick**, D.A. Carter, A. Salazar

CHED **466.** Molecularly imprinted polymers for dopamine recognition. **T. Cheek**, G. Mwangi

CHED **467.** Dietary effects on urinary sulfate levels in pigs measured by a conductometric method. **J. Garcia**, T.A. Parker, K.A. Guay, L.D. Schultz

CHED **468.** NMR spectroscopy as a screening agent for designer opioids. **M. Chambers**, L. Huang

CHED **469.** How poisonous is milkweed? Spectrophotometric determination of cardiac glycosides in *Asclepias syriaca*. **H.G. Bowler**, M.P. Gonella, M.A. Everest

CHED **470.** Proteomics and transcriptomics: Techniques for the discovery of neuropeptide receptors in the American lobster, *Homarus americanus*. **C.Q. Corban**, P.S. Dickinson, A.E. Christie, E.A. Stemmler

CHED **471.** Quantitation and characterization of anthocyanins in medical cannabis flowers cultivated in eastern Oregon. **D. Spikerman**, B. Mandella, R. Hunt, J. Riggle

CHED **472.** Surface-enhanced fluorescence enhancement studies on silver dendrites. **D. Allen**, D. Rios, T. Shtoyko, S. Raut, I. Gryczynski

CHED **473.** Forensic discrimination and quantification of EDTA in dried bloodstains using diffuse reflectance infrared fourier transform spectroscopy, attenuated total reflectance, and liquid chromatography-mass spectrometry. **C.O. Granger**, **C.E. Witt**, J. McCutcheon

CHED **474.** Polyaniline-gold nanocomposites doped with ferricyanide for electrochemical and optical biosensing measurements. **R. Quezada**, R. West

CHED **475.** Pre-equilibration affinity capillary electrophoresis method to probe molecular interactions of heparin to histidine. **A. Schrader**, A.K. Korir

CHED **476.** Analysis and quantification of microbeads in commercial products and the environment through FTIR spectroscopy. **J. Strickler**, G.P. Foy

CHED **477.** Quantitative analysis of chloride concentrations by a chloride ion selective electrode and ion chromatography in southeastern Wisconsin. **M. Tveit**, C.A. Blaine

CHED **478.** HPLC-UV and LC-MS analysis of resveratrol and piceid isomers in Japanese knotweed. **J. Luchetta**, D.E. Mencer, W. Terzaghi, K. Klemow, M. Yatison, D. Pupaza, A. Mikolon, A. Ford

CHED **479.** Analyzing the levels of mercury (Hg) in rice and rice products consumed by residents and students in St. Lawrence County New York. **J. Wilson**, N. Gao

CHED **480.** Identification of individuals by gas chromatography-mass spectrometry analysis of fingerprint residues. **T. Kuhns**, **S. Zentz**, R. Thomas, K. Sarago, J. Saffle, M. Akers, D.S. Egolf

CHED **481.** Qualitative determination of the adherence of VOCs to building materials. **J. Turner**, C.H. Lisse

CHED **482.** Stability of AH-7921 in polar organic solvents. **M. Murphy**, H.L. Ciallella, K. Scott

CHED **483.** Method development for analyzing vibrational modes of unattached violin plates. **M. Flesch**, J. Rollison, C. Hanson

CHED **484.** Stability of synthetic cathinones in beverages. **L. Rutter**, K. Scott

CHED **485.** Analysis of heat dried blood stains through forensic blood testing and DNA profiling techniques. **B. Bosley**, M. Wright, F.L. Musko

CHED **486.** Surface enhanced Raman spectroscopy using silver and gold nanoparticles. **E.S. Breeden**, L.H. Rickard

CHED **487.** Vibrational spectroscopy studies of the role of water in metal ion extraction into room-temperature ionic liquids. **M.L. Rigney**, M.L. Dietz, C.A. Hawkins

CHED **488.** NMR investigation of the effect of pH on micelle formation by an amino acid-based surfactant. **G. Rothbauer**, E. Rutter, F.H. Billiot, E. Billiot, Y. Fang, K.F. Morris

CHED **489.** Method development for analyzing vibrational modes of violins throughout construction process. **J. Rollison**, **M. Flesch**, C. Hanson

CHED **490.** Use of membrane fusion to understand the role of lung surfactant protein B in lipid trafficking. **K. Kroning**, O.H. Braide

CHED **491.** Identification of pigments and the level of degradation in the painting Saint Peter. **D. Seigneur**, S.J. Gravelle

CHED **492.** Detection of date rape drugs in hair using supercritical fluid extraction and gas chromatography/mass spectrometry. **J. Knudsen**, G.P. Foy

CHED **493.** Benchtop deposition of patterned thin films of pentacene. **R. Mendoza**, **N. Rowland**, M.V. Lee

CHED **494.** Influence of salt on the stability of oil-in-water emulsions containing whey protein-xanthan-locust bean complexes. **K.R. Griffin**, **M. Krempel**, H. Khouryieh, K. Williams

CHED **495.** Analysis of metal content of red wines from the winemaking process by ICP-OES. **S. Kvasnovsky**, G.P. Foy

CHED **496.** Cavity ring-down spectrometry of gas-phase ions prepared via electrospray ionization. **B. Rose**, L.A. Ligon, T.G. Spence

CHED **497.** Supercritical fluid and organic extraction and liquid chromatographic-UV/Vis analysis of stevioside from *Stevia Rebaudiana* leaves. **L.R. Stauring**, G.P. Foy

CHED **498.** Electrochemical studies of ferrocenyl chalcones immobilized in Nafion®. **A. Molina-Villarino**, J.C. Aponte-Santini, I. Montes, A.R. Guadalupe-Quiñones

CHED **499.** Electrochemical water quality analysis of the Susquehanna River and Laurel Hill Creek. **S.J. Sujansky**, K. Rublein, L.K. Lee

CHED **500.** Comparison of methods for the capture of e-cigarette emissions for the determination of constituents using gas chromatography-mass spectrometry. **C. Cummings**, M. Bida, A.G. DiFrancesco, I. Rahman, R.J. Robinson, T.E. Pagano

CHED **501.** Top-down and bottom-up proteomics for the identification of crustacean neuropeptides and precursor-related peptides predicted by transcriptomics. **J.M. Michels**, C. Rivera, P.S. Dickinson, A.E. Christie, E.A. Stemmler

CHED **502.** Deposition of nickel nanoparticles on carbon nano-onions via the rotating disk slurry electrodeposition technique for non-enzymatic glucose sensing. **J.J. Soto Perez**, C. Vélez, C.R. Cabrera

CHED **503.** Sensitivity comparison of GC-MS and GC-FID/ECD. **S. Salske**, K.E. Molter

CHED **504.** Construction and alignment of a total internal reflection fluorescence microscope. **K. Griffith**, K. Fogarty

CHED **505.** Withdrawn.

‡ *Cooperative Cosponsorship*

CHED **506.** Identification and characterization of Plutonian and Titan tholins via LDMS and ^{15}N NMR. **J. Nederhoff**, D.V. Kravchuk, M. Flesch, J. Sebree, C. Hanson

CHED **507.** Quenching of electrochemiluminescence in aqueous solution by nitrate explosives. **K.A. Abrams**, K.D. Sienerth

CHED **508.** Determination of heavy metals in CoverGirl and Bare Minerals cosmetic product. **J. Litz**, K. Chichester

CHED **509.** Spectroscopic and spectrometric analysis of two illuminated manuscripts from the 15th and 16th centuries. **B.R. Wydra**, A.M. Fleshman

CHED **510.** Characterization of reactions responsible for aging in wood-based pyrolysis oil. **L.R. Nguyen**, J. Joseph, M.J. Rasmussen, P. Speight, B.G. Frederick, E.A. Stemmler

CHED **511.** Analysis of complex molecules utilizing a 60 MHz FT NMR: How far can we push the magnet? **A. Quintero**, T. Munguia

CHED **512.** Evaluation and refinement of the procedure used to prepare training samples for arson detection K-9s. **E.A. Chance**, **S.D. Oo**, D.W. Carpenetti

CHED **513.** Analytical methods for characterization of synthesized gold nanoparticles in nonpolar solvents. **S. Bonson**, N. Orloff, P.J. Kreke

CHED **514.** Extraction of pesticides in local and imported fruits followed by GCMS analysis. **K. Greeley**, C.D. King

CHED **515.** Second step dissociation constant (pK_2), and related thermodynamic quantities of TES buffer from 5 to 37˚C. **Y. Kang**, T. Wehmeyer, R.N. Roy, L. Roy

CHED **516.** Forensic analysis of trash bags: Microscopical discrimination of trash bags. **D. Daley**, M. Clothier, W. Rowe

CHED **517.** Aptamers as versatile probes for small-molecules and nucleic acids. **A. Gee**, M. de Pina, N. Hughes, D. Daley, M.F. Ali

Section I

Moscone Center

Hall D

Undergraduate Research Posters

Biochemistry

Cosponsored by BIOL and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **518.** Determination of the menstrual cycle's effects on hemoglobin levels. **A.K. Perry**, P. Faber

CHED **519.** Directed evolution of the haloalkane dehalogenase from *C. crescentus*. **M. Ahsan**, E.C. Mundorff

CHED **520.** Withdrawn.s

CHED **521.** Engineering firefly luciferase for improved bioluminescent imaging. **C. Morrissey**, **C. Fick**, A.M. Leconte, T.S. Wu, E.A. Warner, M. Liu

CHED **522.** Sucrose metabolism in kombucha tea. **P.R. Cheek**, J. Inlow

CHED **523.** Investigation into the binding of recombinant intimin and translocated intimin receptor proteins involved in infection by enteropathogenic and enterohmorrghagic *E.coli*. **C. Redmond**, L. OBrien

CHED **524.** Effect of peptide conformational change to a solvent diffusion rate in a silica sol-gel matrix. **R. Sah**, E. Esquivel, R. Singh, K. Smyth, K. Yokoyama

CHED **525.** Towards a bacteria retardant implant surface. **A.A. Schultz**, E.S. Gawalt, N. Reger

CHED **526.** Extraction and identification of vitamin K_2 from black cohosh. **A. Jones**, P.S. Biser

CHED **527.** Preventing gene expression through the interruption of DNA binding. **O. Perdue**, A. Stewart, A. Murray

CHED **528.** Characterization of in vitro amyloid fibril formation from bovine serum gamma globulin using thioflavin T fluorescence and polyacrylamide gel electrophoresis. **C. Schieffer**, M.E. Lee

CHED **529.** Expression of ERα and ERβ in hippocampus and amygdala during altered energy states between sexes. **M. Bhardwaj**, S. Marshall, K. Krolick, H. Shi

CHED **530.** Drug adsorption to spherical supported lipid bilayers. **J. Yin**, A.A. Fuller, G.Y. Stokes

CHED **531.** Effects of amyloid beta oligomers on the oxidation of lipids. **S.E. Cuddeback**, K.M. Matera

CHED **532.** Stabilization of Aβ peptide aggregates using phenolic compounds. **I.R. O'Leary**, K.M. Matera

CHED **533.** Validation of downregulated genes and putative tumor suppressor genes in pancreatic cancer using quantitative reverse transcriptase-PCR. **W.W. Andersen**, A. Smith, K. Dhanwada, N. Goonesekere

CHED **534.** Adenovirus mediated delivery of an engineered DNA sequence for pancreatic cancer treatment. **T. Becker**, M.A. Kennedy

CHED **535.** Expression and purification of glutathione reductase of *Plasmodium falciparum*. An antimalarial drug target of Methylene Blue (MB). **R. Mownn**, H. Prieto

CHED **536.** Early detection of pancreatic cancer. **A. Rivers**, M. Veite, M.A. Kennedy

CHED **537.** Sunscreen chlorination alters its absorptive properties. **A.A. Pohl**, G.H. Purser, R.J. Sheaff

CHED **538.** Effects of chromium-binding peptide on enzymes of the insulin signaling cascade. **L.C. Scott**, P.E. White, J.B. Vincent

CHED **539.** Determining binding affinity of complement factor C1q and prion protein: Implications in down-regulating prion expression on Follicular Dendritic Cells. **G. Bourne**, G.F. Burton

CHED **540.** Enzymatic hydrolysis of 2,2-diphenylethyl glucosinolate. **C.A. Klingaman**, **M.J. Wagner**, J.R. Mays

CHED **541.** Withdrawn.

CHED **542.** Chemical and bioactive capability of twenty mushroom species from the Lower Rocky Mountain region. **O.Z. Schaefer**, A. Leontyev

CHED **543.** Comparing self-assembled monolayers on gold sensor chips for surface plasmon resonance analysis. **A. Forderhase**, J.R. Williams

CHED **544.** Use of thioredoxin solubility tag on lysyl oxidase: Effects on activity and solubility. **A. Hussain**, K.M. Lopez

CHED **545.** Coupling qPCR to split aptamer ligation for the detection of steroid targets. **K. Jones**, E. Kimbrough, J.M. Heemstra

CHED **546.** Membrane assisted polymerization of amino acids. **B. Malley**, S.E. Maurer

CHED **547.** Investigations of the effects of copper(II) on *Pencillium spinulosum chitinase activity*. **B.J. Trujillo**, M. Cruz, S. Walker, S.J. Bonetti

CHED **548.** Characterization of recombinant ENL YEATS domain and its protein-protein interaction with Paf1. **E. Peltan**, S.M. Grigsby, Z. Nikolovska Coleska

CHED **549.** Identification of CDK and VEGFR inhibitors for the treatment of vascular pathologies. **M. Ismail**, V.C. Miles, U. Chaudhry, A. Ahmad, E. LeMelle, H. Conway, K. Lam, T. Walden, R. Komati, M. Bratton, M. Mottamal, G. Wang, H. McFerrin, J. Sridhar

CHED **550.** Characterization of dilated cardiomyopathy linked R25 mutants of phospholamban. **M. Exline**, K. Ha

CHED **551.** Effects of N-terminal disease mutations on HspB1 polydispersity. R. Klevit, A. Clouser, **T.H. Chu**

CHED **552.** Magnetic silicone nanospheres for *in vivo* drug delivery. **K. Pieri**, B. Evans

CHED **553.** Porphyrin-based Photodynamic Antimicrobial Chemotherapy (PACT) and its effects on various bacterial morphologies. **J.A. Smith**, C.E. Stilts, A.M. Wilson, E.A. Dano, J.P. Rynders

CHED **554.** Synthesis of novel cell-penetrating sequences with selective binding to Helix 69. **A. Abu-kwaik**, C.S. Chow, H. Seo, N. Muthunayake

CHED **555.** Characterization of a human G protein-coupled receptor. **M. Doleschal**, T. Frielle

CHED **556.** Expanding the NMR metabolome with enriched and improved growth media. **K. McMahon**, F. Bhinderwala, R. Powers

CHED **557.** Investigation of structure/function relationships in the retaining glycosyltransferase MshA from *Corynebacterium glutamicum*. **C.M. Petersen**, P.A. Frantom

CHED **558.** Solubility studies of a zinc-finger antiviral protein cloned with and without solubility tag. **R. Sargsyan**, D. Lawrence

CHED **559.** Sugar metabolism in cells lacking the tumor suppressor p27kip1. **E. Loe**, R.J. Sheaff

CHED **560.** Synthesis of solvatochromic probes to label the mycobacterial cell wall. **A. Utz**, S. Keyser, C.R. Bertozzi

CHED **561.** Expression and purification of DPAP-1. **D. Coleman**, H. Prieto

CHED **562.** Designing a plasmid to study long range oxidation in DNA. **M. Safaeipour**, **K. Hernandez**, P. Lee, E. Stemp

CHED **563.** Incorporation of nonpolar porphyrin molecules into liposomes. **S.N. Khayyo**, P.K. Kerrigan, **J. Batarseh**, A. Novaj, S. Maio, R. Guglielmo, V. Khayyo

CHED **564.** Characterization of Malaria DHFR Mutants. **S. Akhlaq**, H. Prieto

CHED **565.** Quantification of DNA products using ion-pair reverse phase liquid chromatography. **H. Wienkers**, M. Bestwick

CHED **566.** Determining amyloidogenicity of Islet Amyloid Polypeptide (IAPP) across mammalian species. D.A. Moffet, **E. Njoo**, **D. Rinauro**, **S. Pilcher**, **L. Palato**, B. Johnstone, **K. Menefee**, **A. Tun**

CHED **567.** Targeting cells lacking the p27kip1 tumor suppressor using metformin. **S. Sullivan**, R. Khattab, R.J. Sheaff

CHED **568.** Effects of macromolecular crowding on the inhibition of malate dehydrogenase. **K. Wilber**, D.W. Seybert

CHED **569.** Role of nitroxides in mitochondrial oxidative stress. **M. Abdulrahim**, T.E. Goodwin, A.A. Caro

CHED **570.** Effect of oleocanthal extract from extra-virgin olive oil on the aggregation of amyloid-beta proteins. **A. Cicchini**, M.A. Fisher

CHED **571.** Expression of myxoma virus leukemia-associated protein in the presence and absence of solubility tags. **R. Zietoon**, D. Lawrence

CHED **572.** Using *C. elegans* as a model for avolition. **H. Sumner**, **J. Scott**, K. Weeks

CHED **573.** Role of the eIF2 kinase PERK on whole body and hepatic stress responses to dietary methionine restriction. **C. Kerber**, A. Pettit, T. Anthony, E. Mirek

CHED **574.** Engineering Taq polymerases for the reverse transcription of 2' modified DNA. **E. Lewis**, S.L. Rosenblum, H.E. Chia, A.M. Leconte

CHED **575.** Enzyme folding improves catalytic activity of enzyme cargos in virus-like particle nanoreactors. **A. Hernandez**, D. Patterson, C. Hjorth, J. Bird, T. Douglas

CHED **576.** Cloning and expression of *Pseudomonas aeruginosa elastase in E. coli* for examining inflammatory response of lung tissue. **C. Hjorth**, D. Draper, A. Hernandez, J. Bird, A. Azghani, D. Patterson

CHED **577.** Using site-saturation mutagenesis to identify residues that contribute to cephamycinase activity in class C beta-lactamases. **S. Kim**, S.T. Lefurgy

CHED **578.** Investigating *B. fungorum* antibiotic resistance with transposon mutagenesis. **L. Wethekam**, K.M. Specht

CHED **579.** Cytochrome c's role in a putative apoptosis pathway of *P. falciparum*. **M. Yilmaz**, H. Prieto

CHED **580.** Investigating the diversity of antibiotic resistance genes in cultures derived from activated sludge bacterial communities following exposure to low doses of triclosan. **B. McGivern**, J. Beni, T. LaPara, J. Donato

CHED **581.** Ficoll induced aggregation in bovine serum albumin and not B-phyceorythrin. **K. Blake**, H. Boukari, M.J. D'Souza, Z. M'rah, E. Jhamba

CHED **582.** Exploring the interactions of cytochrome c with diacylphosphatidylglycerol lipids. **B.M. Abbott**, J.J. Breen

CHED **583.** Retinoic acid receptor gamma reciprocally regulates cellular adhesion and proliferation in K562 cells. **V. Niedzwiedz**, **R. Mayo**, M.D. Kelley

CHED **584.** Analysis of the NF-κB transcription factor in the endangered coral *Orbicella faveolata*. **E.G. Salas**, L. Williams, T. Gilmore

CHED **585.** Role of phosphorylation in lipid droplet protein activity. **P. Stangl**, A.K. Stoeckman, D. Mashek

CHED **586.** Synthesis of syndecan 1 vector and its effect on the metastasis signal. **N. Nemmers**, D.C. Speckhard

CHED **587.** Withdrawn.

CHED **588.** Experimental measurements of protein electrostatics in GFP using vibrational stark effect spectroscopy. **D. Fernandez**, C. Lum

CHED **589.** Role of IL-17a in fecal microbiota transplant mediated clearance of *C. Difficile infection*. **M.S. Saffern**, E.G. Pamer, M.C. Abt

CHED **590.** Math anxiety and cortisol as a biomarker. **M.A. Davis**, **C. Lechak**, D. Bateman

CHED **591.** Protein dynamics in Superoxide Dismutase (SOD1). L. Cervantes, **E. Healy**

CHED **592.** Analysis of novel inhibitors of *Borrelia burgdorferi* BGP protein: Potential new antibiotics to treat lyme disease. **T. Firica,** E. Lines, J. Gonzalez, S. Schwarz, J.H. Thurston, D. Xu, K. Cornell

CHED **593.** Analysis of microbial changes in the human oral cavity. **Z. Weiss**, K. Opel, D. Singleton, B. Gray

CHED **594.** Investigations of the unique farming behavior of *Dictyostelium discoideum*. **M. Van Horn**, **L. Morris**, P.L. Kuhlman

CHED **595.** Analysis of emergent electronic properties of self-assembling nucleopeptides. **S. Brown**, S. Singh, P. Patra, J.E. Smith-Carpenter

CHED **596.** Specifically targeting cells lacking the tumor suppressor p27kip1 using metabolic inhibitors. **J. Paracka**l, R.J. Sheaff

CHED **597.** Evolution of membrane stability in the origins of life. **T. Zaniewski**, S.E. Maurer

CHED **598.** Gas chromatography-mass spectrometry analysis of oxidation-reduction products of cholesterol in M624 human melanoma cells. **A. Garlow**, K.S. George Parsons

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

CHED **599.** Identification of Nonribosomal Peptide Synthetase (NRPS) enzymes to find naturally occurring secondary metabolites. **J. Kolasinski**, W. Lloyd, J. Donato

CHED **600.** Detection and analysis of glyoxylic acid uptake in *Calliphora vomitoria* larvae. **H. Byczynski**, A.L. Smalley

CHED **601.** Design of dimethoxytrityl derivative to improve the selectivity in RNA phosphoramidite. **A.M. Hodge**, V.K. Dunlap

CHED **602.** Broadening the scope of sortase-mediated ligations using natural sortase homologs. **N. Horvath**, K. Nikghalb, J. Prelesnik, P. Filipov, J. Antos

CHED **603.** Apoptotic cascade: The role of metal ions on caspases. **C.C. Williams**, M. Davis Mcgibony

CHED **604.** Effects of chelation of Fe(II) and Fe(III) by melanin films on electrochemical characteristics for Parkinsonism disease applications. **C. Schinnerer**, G. LeBlanc, G. Ludewick, H. Fisher

CHED **605.** Determination of phosphorylation site on Vascular Endothelial cadherin (VE-cadherin) using mass spectrometry. **M. Dolan**, C. Minogue

CHED **606.** Interaction of a water-soluble porphyrin with various DNA sequence: A spectroscopic study. **M.K. Wright**, J. McCue, S.M. Basu

CHED **607.** Measurement of beta-oxidation catalyzed by lipid bodies of *Brassica napus using HPLC*. **C.M. LaRussa**, G.A. Giles

CHED **608.** Structural analysis of neurotransmitter-stabilized Aβ oligomers. **M. Allnutt**, K.M. Matera

CHED **609.** Cytotoxicity of novel napthoquinones. **A. Rowe**, J. Alao, J.C. Dicesare, R.J. Sheaff

CHED **610.** Altering the conformational ensemble of the calmodulin binding protein PEP-19. **D. Ordonez**, N. Rathke, C. Mitchell, T. Dunlap

CHED **611.** Deoxyribozyme Sero1C and photoreversion of cytosine dimers. **R. Sapia**, Y. Gerasimova

CHED **612.** Catalytic activity and thermal stability of chymotrypsin encapsulated in self-assembled lithocholic acid nanotubes. **L. Stiff**, Q. Lu, G.E. Collins, R.L. Siefert

CHED **613.** Interaction points between stromally exposed CpTatC and precursor signal peptide. **G. Thomas**, A. Habtemichael, C. Dabney-Smith

CHED **614.** Characterization of jhp0715, a putative member of the futalosine pathway in *Helicobacter pylori*. **C. Khalil**, A. Roberts

CHED **615.** Investigation of the structural features necessary for a positive THC assay. **Z. Zhou**, C. Lassiter, B.L. Martinez

CHED **616.** Investigation of human pol eta's role in translesion synthesis past cisplatin-induced DNA damage. **K. Bryson**, S. Lone

CHED **617.** Synthesis of chitosan coated nanodiamonds to prevent *Staphylococcus aureus* and *epidermidis* infection in bone implants. **P.O. Méndez**, E. Nicolau, J. Santillan, V. Ortiz, Y. Rodríguez

CHED **618.** Development of an undergraduate peptide synthesis lab for organic and biochemistry courses. **S. Bingaman**, **B.M. Day**, **J.F. Larrimore**, M.J. Crawford

CHED **619.** Cloning isoprenoid synthesis genes from *Thermoplasma volcanium* using the FX-cloning method. **O. Blomquist**, C. Banach, J.A. Himmelberger

CHED **620.** Withdrawn.

CHED **621.** Impact of BosR mutations on its DNA binding properties. S.E. Evans, **D. Xenos**

CHED **622.** Development of a sensitive assay to detect tRNA modifications in cell culture. **J.B. Mamaril**, T.R. Vornheder, J. Burchett, M.P. Guy

CHED **623.** Characterization of a terpene synthase from *Fischerella muscicola* PCC 9339. **S.D. Knapic**, M.L. Hillwig

CHED **624.** Examining the effect of insulin on membrane association of islet amyloid polypeptide. **E. Hegedus**, M. Gessel

CHED **625.** Characterization of a haloacid dehalogenase superfamily enzyme from *Mycobacterium tuberculosis*. **G. Kaur**, A. Roberts

CHED **626.** Development of a fluorescence assay for the evaluation of nucleotide-analog incorporation during the elongation stage of RNA synthesis by hepatitis C virus NS5B RNA polymerase. **M.N. Kenyon**, M.L. Hillwig

CHED **627.** Withdrawn.

CHED **628.** Differential carbon metabolism in cells lacking the tumor suppressor p27kip1. **K. Counter**, R.J. Sheaff

CHED **629.** Directed evolution of haloalkane dehalogenase from *Caulobacter crescentus* towards smaller, chlorinated substrates. **M. Rahman**, **Y. Xiong**, E.C. Mundorff

CHED **630.** Low level DNA analysis from public and private surfaces by real time PCR. **C. Bowman**, K. Opel

CHED **631.** Macromolecular crowding effects on Lactate Dehydrogenase (LDH). **S.A. Shaik**, D.W. Seybert

CHED **632.** Withdrawn.

CHED **633.** Imatinib activity against cells lacking the tumor suppressor p27Kip1. **A. Lignieres**, R.J. Sheaff

CHED **634.** Analysis of carbohydrates in the beer brewing process using HPLC. **K. Alderfer**, N. Fresco, J.A. Himmelberger

CHED **635.** Development and identification of affibody molecules that target crotalid snake venoms. **A.F. Sullivan**, **M. Sudduth**, K.A. Noren, C.J. Noren, E. Osborne

CHED **636.** Characterization of methylenetetrahydrofolate reductase oligomers utilizing hydrogen/deuterium exchange coupled with liquid chromatography and mass spectroscopy. **C. Jeon**, E.E. Trimmer, E.M. Marzluff

CHED **637.** Investigating mycobacterial L,D-transpeptidases in cell wall biosynthesis. **R.L. Marshburn**, L. Basta

CHED **638.** Applying FRET to quanitfy dimer swapping in the auxin signaling pathway. **M. Chiriboga**, K. Piemonte, O. Chaarawi, J.P. Ellis

CHED **639.** Analysis of mutations in *E. Coli* carbamoyl phosphate synthetase I. **B.J. Davis**, B.A. Smith

CHED **640.** Biological effects and chemical aspect of Peruvian teas. **S. Jimenez**, **E. Davis**, L. Nogaj, S. Deprele

CHED **641.** Aggregation mechanisms of amyloid-beta and insulin. **V. Grove**, K.M. Matera

CHED **642.** Effect of combination disulfiram-copper treatment on ARV-7 expression in castration-resistant prostate cancer. **Y.K. Elghoul**, Q. Dou

CHED **643.** Synthesis of a series of 2-acetyl-thiazole thiosemicarbazone ligands and their characterization by NMR spectroscopy and MIC studies. **A.K. Buckner**, A.R. Nesbitt, E.C. Lisic

CHED **644.** Investigation of varying metal organic frameworks for the use as a slow release mechanism for insulin. **W. Adrian**, Z. Mensing

CHED **645.** Oxidative DNA-protein crosslinking induced by oxidation of 8-oxoguanine by $Os(phen)_2dppz^{3+}$ via the flash-quench technique. **M. Safaeipour**, E. Kroll, **J. Dominguez**, E. Stemp

CHED **646.** Classifying the mode of inhibition of DNA methyltransferase inhibitors. **J. Hoover**, M.A. Fisher

CHED **647.** Biological characterization of novel napthoquinones as potential chemotherapeutics. **R. Bacani**, J. Alao, J.C. Dicesare, R.J. Sheaff

CHED **648.** Investigation of the structure and function of P-Rex2: Implications for a molecular mechanism of PTEN inhibition. **T. Diethrich**, D. Needle, S.M. Ensel, D.S. Waugh, G. Miller

CHED **649.** Insulin effects on cell metabolism in cells lacking the tumor suppressor p27kip1. **R. Khattab**, S. Sullivan, R.J. Sheaff

CHED **650.** Expression of antioxidants in CMV infected heart cells. **I. Naron**, K. Weeks

CHED **651.** Characterization of potential allosteric effectors of bacterial MTN. **K.R. Bertagnolli**, S. Nick, P. Erstad, D. Xu, J.H. Thurston, K. Cornell

CHED **652.** Effect of vitamin D3 on paclitaxel potency in triple negative breast cancer cell lines. **C. Wilhelm**, J. Kelts

CHED **653.** Use of budding and fission yeast to study the roles of eukaryotic tRNA modifications. **T.R. Vornheder**, M.E. Thomas, K. McElheney, S. Russell, **M.P. Guy**

CHED **654.** Systematic analysis of mechanisms of small heat shock protein function in *Dictyostelium discoideum*. **B. Lyda**, K.M. Scaglione, J. Bruns Scaglione

CHED **655.** Validation of qPCR rapid bacterial quantification through viable *E. coli cell count in the Saginaw Bay Watershed*. **T. Lefevre**, T. Sivy

CHED **656.** Using a fluorescent probe to monitor DNA photoadducts. **L. Lin**, N.J. Greco

CHED **657.** Synthesis and photophysical evaluation of 6-aryl-2'-deoxyuridine nucleosides. **F. Balarezo**, N.J. Greco

CHED **658.** Interactions of the fragile X mental retardation protein with BACE1 mRNA and miR-124-3p. **P. Zakutansky**, M. Mihailescu

CHED **659.** Exploring the role of Gln120 in *Enterobacter cloacae* P99 cephalosporinase by site-saturation mutagenesis. **A. Brodovskaya**, S.T. Lefurgy

CHED **660.** Incorporation of 3'OMe-NTP by mutant DNA polymerases. **A. Weiden**, H. Schultz, H.E. Chia, S. Rosenblum, A.M. Leconte

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CHED **661.** Biophysical investigation of DNA local structure. **L. Radford**, **I.O. Okeke**, M. Hatcher

CHED **662.** Heme pocket interactions with fluoride in the hemoglobins from *Lucina pectinata*. **K. Frankenfield**, K. Williams, D.M. Rivera, J. Lopez Garriga, J. Cerda

CHED **663.** Effect of the plant polyphenols on CYP2E1-dependent oxidative stress. **N. Horan**, A.A. Caro

CHED **664.** Role of copper and tor signaling in reactive oxygen species induced cell aging. **M.E. Walser**, M. Bestwick

CHED **665.** Effect of mitochondrial CYP2E1 overexpression on mitochondrial oxidative stress in HepG2 cells. **P. Gitz**, **A.A. Caro**

CHED **666.** Quantification of the in vitro inhibitory effects of the Erythrina crista-galli lectin on HIV-1 reverse transcriptase. **M. Vazquez Camacho**, R. Ynalvez

CHED **667.** Effect of exogenous testosterone administration on blood DHT levels and prostate hyperlasia in adult male mice. **J. Angelillo**, B.A. Davis

CHED **668.** Monitoring *htrA* RNA thermometer activity using a β-galactosidase assay in *Escherichia coli*. **Y. Nguyen**, R.M. Mitton-Fry

CHED **669.** Quantifying risk factors for Alzheimer's disease using neuroimaging data. L.D. Bienski, O. Alzate, L. Smith, **R. Barbosa**, **L. Rattanavong**

CHED **670.** Selectivity of protein sulfhydration. **T. Johnson**, C. Kevil, X. Shen

CHED **671.** Analysis and assignment of the ^{1}H-^{15}N HSQC of the PDZ-1 domain from zonula occludens protein 1. **L. Morin**, M. Wheelock, T. Steele, A. Long, A.L. Jansma

CHED **672.** Expression of a membrane protein mutant in *Burkholeria cenocepacia*. **C. Barcelo**, K.M. Specht

CHED **673.** G-qudruplex specific ligands attenuate supramolecular G-DNA assembly. **E.M. Kalb**, T.C. Marsh

CHED **674.** Role of metformin binding in reducing the extent of nonenzymatic glycation of albumin. **A. Jensen**, M. Finkbeiner, S. Becker, R.W. Holman, K. Rodnick

CHED **675.** Stimulation of human 8-oxoguanine DNA glycosylase by AP endonuclease: Effect of polymorphisms. E. Klein, **K.A. Haushalter**

CHED **676.** Effects of Δtor1 on yeast longevity via chronological lifespan assay. **A. Keyes**, M. Bestwick

CHED **677.** Nanoscale modifications to the RsaA S-layer protein enhance lead binding in whole cells. **A. Coblentz**, **K. Templeton**, E. Bailey, C. DeAlba, W. Jenkins, J.A. Cappuccio

CHED **678.** Binding of small aromatic molecules to phytochemical capped gold nanoparticles. **N. Anderson**, M.A. Fisher

CHED **679.** Antibacterial activity studies of 2-[[4-(1-methylethyl) phenyl] methylene]-hydrazinecarboxamide in *Escheria coli*. **K. Fernandez**, T. Munguia

CHED **680.** Effects of membrane composition on pore-forming polypeptides. **Z. Maxwell**, S. Swain, M. Gessel

CHED **681.** Electrochemical studies of L-cysteine /zinc interactions in aqueous media. **M. Doan**, G.T. Cheek

CHED **682.** Determination of the molecular pathway causing phosphorylation of zonula occludin 1 and disassembly of tight junctions in diabetes. **O. Ogline**, R.L. McCann

CHED **683.** Construction of a His-tagged expression plasmid for sfnaB of the Staphyloferrin A biosynthetic pathway. **C.A. Dombroski**, J. Cederberg, D.J. Schedler, W. Kittleman

CHED **684.** Preparation and purification of a protein kinase inhibitor-GST fusion protein for a bio-layer interferometry binding study. **D. Stoesz**, G. Li, G. Veglia, M.B. Neibergall

CHED **685.** Mechanistic insight into taurine as an anti-glycation agent. **S. Becker**, M. Finkbeiner, A. Jensen, R.W. Holman, K. Rodnick

CHED **686.** Viral silencing suppressor specificity for shared structures of miRNA and siRNA. **A. Whitehill**, J.M. Vargason

CHED **687.** Investigating mycobacterial L,D-transpeptidases in cell wall biosynthesis. **P. Stateler**, L. Basta

CHED **688.** Effect of Peruvian teas on mammalian cells. **D. Morales**, K. Araujo, S. Deprele, L. Nogaj

CHED **689.** Comparison of the iron oxidation mechanisms in heteropolymer ferritins of different H to L ratios. **A. Farghli**, M. Mehlenbacher, B. Smith, M. Poli, P. Santambrogio, P. Arosio, S. Levi, F. Bou-Abdallah

CHED **690.** Effect of the plant polyphenol catechin on CYP2E1-dependent oxidative stress. **C. Schwab**, A.A. Caro

CHED **691.** Characterization of glutathione inhibition of oxidative DNA-protein crosslinking. M. Safaeipour, **J. Jauregui**, **S. Castillo**, M. Bekarian, M. Sanchez, E. Stemp, E. Tiznado

CHED **692.** Characterization of the malA enzyme from B*dellovibrio bacteriovorus* through the synthesis and analysis of maltose and α-methyl-glucopyranoside derivatives. **J. Jepson**, J.E. Hanson

CHED **693.** Evaluation of the generation of superoxide anion by CYP2E1 using the spin probe CPH. **C. Ryan**, A.A. Caro

CHED **694.** Drug binding to cytochrome P450: Sample annealing studies using EPR. **D.W. White**, M. Bowman

CHED **695.** Effect of CYP2E1 overexpression on mitochondrial biogenesis in HepG2 cells. **L. Davis**, A.A. Caro

CHED **696.** Baculovirus expression, amplification, and protein purification of recombinant rat serotonin transporter containing a single point-mutation for future crosslinking studies. **E. Cooper**, E. Castellano, M. Cascio

CHED **697.** Docosahexaenoic acid induces mitochondrial biogenesis in HepG2 cells that overexpress cytochrome P450 2E1. **J. Anderson**, A.A. Caro

CHED **698.** Withdrawn.

CHED **699.** Investigating the growth rate of MntH knockout mutant of *E.coli*. **A. Edobor**, M. Nguyen, B. Cadena, D. Duran, P. Lee

CHED **700.** Metal ion cofactor requirements for snake venom phosphomonoesterase. **I. McVinney**, R.A. Kopper

CHED **701.** Elucidating structure-function relationships of the phosphorylated human protein MEK1 through the integration of biotechnologies. **A. Gallant**, S. Aiello, A. Ringer McDonald, J. Oza

CHED **702.** Inhibition of oxidative DNA-protein crosslinking via vitamin C. **M. Serrano**, M. Martinez, P. Perez, E. Kroll, J. Ordenana, E. Stemp

CHED **703.** Over-expression and purification of *E. coli* recombination protein RecR and its interlocking mutants using various protein chromatographic methods. **S. Koo**, **C. Jaipersaud**, J. Trabucco

CHED **704.** Withdrawn.

CHED **705.** Benefits of floatation tanks as novel tools for stress reduction. **T. Makkapati**, P. Lin, C. Wohlrab, J. Feinstein, A. Alarbi, W. Potter

CHED **706.** Purification of horseradish peroxidase for biochemistry lab. **N. Lo**, A.L. Miller

CHED **707.** Expression, purification, and characterization of codon optimized DszB from *N. asteroides*. **K. Idrizi**, D. Hoang, J. Gumpf, L.M. Watkins

CHED **708.** Structural, enzymatic, and inhibitory study of *M. tuberculosis* Rv3802c. **C.M. Schreidah**, C.M. Goins, D.R. Ronning

CHED **709.** Novel heme-anion complexes of cytochrome c′. **C. Norman**, B.N. Mees, J. Vardenega, C. Mitchell, D. Bedolla Sotelo, B. Mandella, Z. Nilsson, C. Andrew

CHED **710.** Two-dimensional analysis of apolipoproteins using gel electrophoresis and SDS-PAGE. **N.B. Nguyen**, R. Chandra

CHED **711.** Mechanism of oxygen reduction in copper amine oxidases. **K.E. Gazica**, **M.M. Saugstad**, S.A. Mills

CHED **712.** Effect of Ca^{2+} signaling on Rho GTPases during neurogeneration. **J. Tobin**, B. Avery

CHED **713.** Determining which part of the region between the GlnS and ChiP genes downregulates *rpoS* in *Escherichia coli,* TsiR or the 5' UTR of ChiP. **C. Diop**, C. Peterson

CHED **714.** Cloning and expression of the predicted aspartate hydroxylase ORF1 from *Streptomyces verticillus*. **P. Nguyen**, C.T. Calderone

CHED **715.** Synthesis of sulfated sialic acid glycodendrimers to interfere with bacterial biofilm formation. **R. Suasin**, K.D. McReynolds

CHED **716.** Withdrawn.

CHED **717.** In vitro analysis of the thyroid hormone receptor in mitochondrial transcription. **D. LeGrady**, M. Bestwick

CHED **718.** Site-Directed mutagenesis in the rat serotonin transporter. **K. Spirik**, M. Cascio

CHED **719.** Exploration into preventing bacterial adhesion on nitric oxide releasing polymers. **L. Paricio**, B.H. Neufeld, M.M. Reynolds

CHED **720.** Withdrawn.

CHED **721.** Effects of porphyrins as photodynamic agents. **T. White**, J.E. Bradshaw, T.E. Hayes

CHED **722.** Male sex hormones regulate human endothelial nitric oxide synthase system through the modulation of cationic amino acid transporter-1. **L. Levy**, D.W. Estes

CHED **723.** Antibacterial assessment of cyclogossine A, a cyclic heptapeptide from *J. gossypiifolia*. **E. Barksdale**, C.L. Telzrow, A.J. Wommack

CHED **724.** Structural analysis of novel inhibitors through docking of homology modeled yeast α-glucosidase. **J. Turner**, S. Kennedy

CHED **725.** Investigating inhibitor resistance to proteasome subunit Rpn13. **T. Engdahl**, P. Dickson, T.J. Kodadek

CHED **726.** Proteases in venomous snake species of Arkansas. **A. Katke**, R.A. Kopper

CHED **727.** Developing an efficient method for the incorporation of a series of fluorotyrosines in peptides via solid phase peptide synthesis. **N. Chau**, A. Colla, J.P. Schwans

CHED **728.** Analysis of UV degradation of amino acids in membranes. **R. Bowman**, S.E. Maurer

CHED **729.** Pulse amplitude modulation fluorometry as a means to determine photosynthetic modes of *Chlorella vulgaris*. **P.E. Adkins**, D. Kolling, B. Woodworth, A. Holland, A. Stevenson

CHED **730.** TEV mutant production. **L. Hongsermeier**, D.C. Speckhard

CHED **731.** Analysis of tyrosinase inhibition with extracted catechins from granny smith apples. **S. Maxwell**, R.E. Rigsby

CHED **732.** Biosynthetic study of the formation of the azinomycin epoxide moiety. **M. Antoniv**, C. Watanabe

CHED **733.** Engineering metalloproteins for fuel catalysis using SLiCE and CHIP template. **E. Reale**, J. Kleingardner

CHED **734.** Rationally designing DNA polymerases for 2'-modified DNA synthesis. **S. Rosenblum**, H.E. Chia, E.L. Lewis, M. Liu, M. Cao, A.M. Leconte

CHED **735.** Bacterial growth studies of gut microbes including *Lactobacillus rhamnosus GG* and *Escherichia coli HS* using UV-VIS spectrophotometry and Quantitative PCR (QPCR). **D. Parikh**, K. Djambazova, P. Aggarwal, S. Kim

CHED **736.** Expression of perilipin 2 in *Escherichia coli* and purification by nickel affinity chromatography. **A. Clements**, A.K. Stoeckman, C. Najt, M.B. Neibergall

CHED **737.** Characterization of 1-amino-9,10-anthraquinone in the A_1 site of PS I complexes of the plastoquinone-containing mutants of *Synechocystis sp. PCC 6803*. **A. Montoya**, P. Kerns, E. Gosselin, T.W. Johnson

CHED **738.** Redox regulation of plasmid copy number and conjugative transfer. **A. Bruefach**, B. Buttaro

CHED **739.** Structural investigations on ER membrane complex subunit 9. **S. Conticello**, C. Murphy, **K.R. Gallagher**

CHED **740.** Development and analysis of a novel protein fusion system for the expression and purification of proteins. **C.G. Toomey**, C. Chant, A. Chant

CHED **741.** Methods of expresion and purification of PEP-19: A calmodulin binding partner. **C.D. Mitchell**, T. Dunlap

CHED **742.** Regulation of tumor suppressor p27kip1 by transglutaminase. **R. Al-Refai**, R. Patel, L. Zhang, R.J. Sheaff

CHED **743.** Inhibition of oxidative DNA damage via green tea. **P. Perez**, M. Serrano, M. Martinez, E. Kroll, J. Ordenana, E. Stemp

CHED **744.** Weight of fatty acids: An examination of a high-fat diet and cognition. **D. Williams**, A. Darkazalli, J. Boggs, L.A. Zuraw, C. Sims-Robinson

CHED **745.** Altering the conformational ensemble of Pep-19 using calcium. **N. Rathke**, T. Dunlap

CHED **746.** Effect of Rad 23 selectivity to polyubiquitin chain linkage on Far-1 degradation in yeast. **Y. Liu**

Section I

Moscone Center

Hall D

Undergraduate Research Posters

Biotechnology

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N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **747.** Preparation and study of protein-based nanotechnology for cost-effective water treatment. **T. Mai**, K. Duran, D. McWhinney, J. Hollingsworth

CHED **748.** Development of a low-cost molecular cloning vector for easy pathway overexpression in *E. coli*. **C. McCutcheon**, J.A. Jones

CHED **749.** Expression in *E. coli* and purification of full-length or partial Medicago truncatula cDNA-encoded Anthocyanin Reductase (ANR) using MBP fusions. **P.S. Whitehead**, **E.P. Landers**, **L. Chandler**, **N.L. Paiva**

CHED **750.** Low-cost modification of a lab scale bioreactor to simulate oxygen gradient heterogeneities present in large scale industrial bioreactors. **A. Armstrong**, I.M. Reizman

CHED **751.** Diversity of predator-escape behaviors and habitat influences on hindlimb skeleton morphology. **A. Biyari**, E. Dewar

CHED **752.** Electronic signatures of nucleobase codons in single-walled carbon nanotubes for rapid genome sequencing. **A. Ortiz**, M. Dorko

CHED **753.** Development of cell based microfluidic devices to study the effect of alcohol on C2C12 muscle cell differentiation. **E.L. Smith**, A. Sarangan, O. Kielbasa, J.E. Smith

CHED **754.** Development of split-protein biosensors for the detection of DNA. **P.V. Halas**, **E.K. Dell**, S.C. Meyer

CHED **755.** Constructing peptide-based molecular building blocks for the controlled assembly of nanomaterials. **J. Bird**, L. Laperriere, H.N. Gray, S.C. Butler, D. Patterson

CHED **756.** Synthesis of functionalized NBD-556 for the binding of HIV-1 gp120 on a solid support. **J. Cuyler**, S.G. Tajc

CHED **757.** Protein-Polymer conjugates using grafting-to and grafting-from approaches. **M. Paeth**, M. Lucius, D. Konkolewicz

CHED **758.** Expression of site-specifically phosphorylated reflectin A1 via an expanded genetic code. **B. Concepcion**, **M. Kamranikia**, R. Levenson, D. Morse, J. Oza

CHED **759.** Metabolic engineering in cyanobacteria: Utilizing quorum sensing to control production of 2,3-butanediol. **J. Beauchamp**, A. Carroll, M. Kanno, S. Atsumi

CHED **760.** Cobalt electron mediators for use in Photosystem-I biophotovoltaics. **M. Alarcon**, N.G. Brady, M. Vaughn, B. Bruce, J.J. Bergkamp

CHED **761.** Biosynthesis of polyhydroxyalkanoate with *Pseudomonas putida*. **M. Cheung**, M. Mendoza, I. Alanis

Section I

Moscone Center

Hall D

Undergraduate Research Posters

Chemical Education

Cosponsored by SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **762.** Learning in the moment: Identifying and improving student conceptual knowledge construction in general chemistry. **B.L. Minshall**, J.H. Torres King, E.J. Yezierski

CHED **763.** Etching of metals by chemical and electrochemical methods: A laboratory activity for middle and high school students. **B.O. Wise**, G.B. Freese, K.W. Kittredge

CHED **764.** Educational study on the use of models to teach molecular shape. **D. Dils**, L. McAfee, B. Adair, L.A. Zuraw

CHED **765.** Guided inquiry approach to design student-friendly coupling methods for 2,2'-bipyridines as precursors for Ru-complexes. **E. Rinaldi**, B. Aukszi

CHED **766.** Quantitative analysis of the impact of classroom salon on introductory chemistry student performance. **B. Walters**, A. Blecking

CHED **767.** Design elements of online learning systems that increase student use and perceptions of optional online study materials. **C. Hansen**, R. Bodily, R. Sansom

CHED **768.** StudentsGiveHope.org: A platform for S.T.E.M. education, inspiration, and student-led medical innovation. B.M. Samudio, **H. Lakkis**, A. Nicholas, C. Billings, F. Abbott, J. Idrovo, J. Schaffer, L. Mergens, M. Lozancich, P. Kim, T. Yamanishi, T. Kirkevold, Y. Lakkis

CHED **769.** Novel stereochemistry experiment for sophomore organic chemistry lab. **A.A. Seba**, **J.E. Blue**, **A. Burns**, H. Hall, C. Nicholson

CHED **770.** Students' perception of how science writing heuristic pre-labs prepare them for lab. **N. Bonde**, D.I. Del Carlo

CHED **771.** Evaluation and improvement of online homework for foundations of inorganic chemistry. **M. Strumolo**, S.G. Sobel

CHED **772.** Examining ink and paper chemistry in middle and high school chemistry. **G.B. Freese**, B.O. Wise, K.W. Kittredge

CHED **773.** Use of *in silico* Structure Activity Relationship (SAR) project in medicinal chemistry course at Winona State University: Molecular docking simulation and analysis of human dopamine D3 receptor-rotigotine analog binding. **T. Provost**, M.E. Lee

CHED **774.** Measuring learning outcomes in chemistry outreach in K-6 elementary school students. **M. Nafea**, M. Tomaraei, R. Mcfarland, R. Ali, P. Robinson, D. West, P.J. Iles, R.V. Valcarce, L.D. Giddings, N.R. Bastian, M. Alvarez, R. Holcomb

CHED **775.** 3-D printed macroscopic model of an atomic force microscope. D. Gruber, **T.J. Perez**, W.J. Miller

CHED **776.** QR codes as a conduit to assess student comprehension of real-world applications of first semester freshman level chemistry concepts. F.M. Yarberry, **S.G. Freyaldenhoven**, M. Massey

CHED **777.** Single vs. mixed approaches to form colored silver nanoparticle films. **H. Skipper**, M. Roca

CHED **778.** Using screencasts and simulations to help chemistry students understand chemical kinetics. **M. Biesbrock**, D.G. Herrington, J.R. Vandenplas, R.D. Sweeder

CHED **779.** Empowering undergraduates to be green chemistry ambassadors through community outreach. **M.C. Enright**, C. Hsu

CHED **780.** Faculty expectations for meaningful learning in the undergraduate chemistry laboratory: How do students' experiences compare? **J. Orzel**, E. Gross, K.R. Galloway, S. Bretz

CHED **781.** Eliciting higher order reasoning in the chemistry laboratory. **K. Collins**, R. Sansom

CHED **782.** Green, cascade synthesis of a grandifloracin precursor: An undergraduate experiment. **G.G. Castro**, D.A. Vosburg

CHED **783.** Impact of chemistry/mathematical video-lectures on student-based learning in a freshman level chemistry course. F.M. Yarberry, **A.H. Stebbins**, L. Christman

CHED **784.** Inter-institutional collaborative chemistry assignments. **T.K. Chasteen**, **C. Egler**, L.A. Morsch, B. McCollum, D. Skagen, B. Shokoples

CHED **785.** Construction of a low-cost LEGO microcomputer controlled visible absoprtion spectrometer. **M. Buell**, D. Albert

CHED **786.** Effect of video-based instruction on student performance in a college chemistry laboratory. F.M. Yarberry, **K. Walden**, M. Massey

CHED **787.** Pedagogical analysis of exam question format of multiple choice or open response in organic chemistry. **K. Tang**, S. Xie

CHED **788.** Examining the connection between what the team members of an interdisciplinary collaboration identified as their goals and how they thought those goals should be evaluated: The ChANgE Chem project. **S. Barakat**, N. Millick, M. Orgill

CHED **789.** Exploring standards and standardization in the physical chemistry laboratory. **M.E. Gasbarre**, B. Ramos, C.J. Hayes

CHED **790.** Thermoelectric generators and Peltier coolers for the physical chemistry teaching laboratory. **J.R. Frey**, R.J. Noll

CHED **791.** Generation of nitrosyl and nitryl halides using heterogeneous reaction chemistry: A spectroscopic and computational project for the physical/atmospheric chemistry laboratory. **T.M. Sytsma**, A. Li, J.A. Ganske

CHED **792.** Heat capacity ratio measurement. **T. Adams**, B. May

CHED **793.** Investigating students' choice of representations for problem solving in organic chemistry. **M. Plekker**, J.R. Vandenplas

CHED **794.** Synthesis of fluorescein and other dyes for spectroscopic analysis. **P. Ruffier**, D.B. Cordes

CHED **795.** Investigating how chemistry teachers change the use of Johnstone's levels in their descriptions of practice during a longer-term professional development program. **N.W. Spurgus**, D.J. Frank, J.M. Pratt, E.J. Yezierski

CHED **796.** Validation of acetaminophen using HPLC, an undergraduate experiment. N. Akanda, **J. Zhang**

CHED **797.** Development of instrumental analysis lab experiment for the determination of organo-arsenic compounds. **S. Goldsberry**, B.M. Hopkins

CHED **798.** Investigation of analgesic separations: A forensic case study. **R. Davies**, A.M. Hupp

CHED **799.** Development of high performance liquid chromatography methods for a Waters Alliance 2695 running Empower 3 software. **S. Shreiber**, T.E. Dermota

CHED **800.** Everything but the kitchen sink! Development of an analytical chemistry capstone lab testing student understanding of course topics. **E. Lewis**, J.A. Goodnough

CHED **801.** Chemistry in television. **C. Albrecht**, S. Wuerz

CHED **802.** Analytical chemistry and public perception. **M. Montes**, S. Wuerz

CHED **803.** Myths and misunderstandings in chemistry. **C. Ryan**, S. Wuerz

CHED **804.** Environmental footprint of drinking water. **C. Aparicio**, S. Wuerz

CHED **805.** Water taste and water quality. **G. Reyes**, S. Wuerz

CHED **806.** Popular understanding of water quality. **L. Parsons**, S. Wuerz

CHED **807.** In-class demonstrations. **A. Koehn**, S. Wuerz

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CHED **808.** Student knowledge of factors for success in chemistry. **S. Barrett**, S. Wuerz

CHED **809.** Filtered available phosphate by FIA: A partnership between chemistry and geology. **J. Onyeagba**, P.J. Iles, R. Kochambilli, L.D. Giddings, R.V. Valcarce, N.R. Bastian, M. Alvarez, R. Holcomb

CHED **810.** Utilizing 3-D printing to enhance classroom instruction of dynamic nature of proteins. **J. Green**, M. Guthrie, L. Manner, J. Bowden, S.S. Ruebush

CHED **811.** Dip coater. **M. Bresnahan**, B. Veldman

CHED **812.** Impact of mindset on the persistence of STEM majors. **J. Hackleman**, B. Brando, A. Stacy, A.M. Baranger

CHED **813.** Connecting dots to community through chemistry at St. Xavier University, Chicago. **P.M. Brehm**, B. Alappat

CHED **814.** Role models and mentors matter for Tennessee girls in STEM. J.M. Iriarte-Gross, **T. Thomas**, K. Owens, R. Marlin, A. Williams

CHED **815.** Synthesis and analysis of fullerenes in the undergraduate physical chemistry laboratory. T.J. Fuhrer, **A. Lambert**, **H. Bell**, **C. Roper**

CHED **816.** Using a ranking task coupled with semi-structured interviews to characterize upper-division chemistry students' modeling practices in quantum chemistry: A mixed-methods study. **C. Crickmore**, M.N. Muniz, J. Beck

CHED **817.** Diffraction: A butterfly experiment. **B.A. Bober**, M.O. McAnally, I. Jones, H. Shi, M. Su, B. Negru

CHED **818.** What chemical facts does the public need to know? **M. Winkelman**, S. Wuerz

CHED **819.** Chemical safety and chemical disposal. **A. Argueta**, S. Wuerz

CHED **820.** Chemical storage in home, shop, and public areas. **J. Montoya**, S. Wuerz

CHED **821.** Magic in chemical education. **A. Morris**, S. Wuerz

CHED **822.** Factor analysis for academic success in chemistry. **B. Claro-Martinez**, S. Wuerz

CHED **823.** Withdrawn.

CHED **824.** Binary liquid-vapor phase diagrams with desktop gas chromatography. B.A. Rowland, **P. Bayliss**

CHED **825.** Philatelic table of the elements as a teaching tool: Topics in health and medicine. **B.T. Winn**, L.G. French

CHED **826.** Implementing preferred VARK learning modalities in organic chemistry. **K. Page**, S.K. Hamilton

CHED **827.** Timing of homework completion vs. performance in general chemistry. **M.N. Cosio**, V.M. Williamson

CHED **828.** Optimize of teaching contents and the develop of teaching methods to the compulsory course of general chemistry in universities. D. Tang, Z. Sun, **Z. Yu**, H. Lv

CHED **829.** Microwave-assisted Fischer indole synthesis for the organic chemistry laboratory. **M. Rico Mendoza**, M.T. Wentzel

CHED **830.** Implementing a flipped classroom and active learning techniques in general chemistry to augment student success at a mid-sized rural university. E. Bladorn, C. Chatha, **V. Cherrette**, H. Dailey, J. Lopez, H. MIlls, C. Park, H. Park, A. Rose, S. Sherry, R. Skorheim, M. Smith, E.C. Wasinger

CHED **831.** Assessing the levels of models upper-division chemistry students develop and apply in the context of the hydrogen atom: A qualitative investigation. **J. Kirsch**, J. Beck, M.N. Muniz

CHED **832.** Effect of online homework on students' performance in introductory chemistry. **H. Syu**, B. Adair, S.T. Mabrouk

CHED **833.** Spinning towards low-cost spin coaters. **H. Speerstra**, B. Veldman

CHED **834.** Biochemistry research in the general chemistry lab classroom: A pilot study. **J. Callus**, S. Juris, K. Spencer, J. Tomasik

CHED **835.** Using analgesia as a theme in the first semester of organic chemistry laboratory. **N. Akanda**, **R. Blough**, **J. Orlandi**, M.J. Castaldi, J.K. Murray

CHED **836.** Computer-aided Design (CAD), fabrication, and testing of an inexpensive 3D printed filter fluorometer. **M.H. Hakim**, **D.A. Rourke**, L.A. Porter

CHED **837.** Conceptual understanding and context: Free energy. **K. Wilson**, J. Nyachwaya

CHED **838.** Role of porphyrins in teaching organic chemistry. **Z.J. Gregg**, J.C. Quirke, J.M. Quirke

CHED **839.** Homemade antacid tablets for the antacid titration lab. **J. Thom**, A. Kwong, W.J. Miller

CHED **840.** Complete binary phase diagram laboratory for undergraduate physical chemistry courses. **T.P. Dorch**, B. Veldman

CHED **841.** Effectiveness of chemical demonstrations in increasing student interest in science. D.G. Watson, Y. Gibson, **M. Taylor**

CHED **842.** Development and implementation of popular diets case studies in a biochemistry course for dietetics majors. **K. Franklin**, **A. Gamez**, **R.M. Hyslop**, **C.E. Brown**

CHED **843.** Prototyping a simple and inexpensive colorimeter from 2D designs via laser cutting and engraving. **H. Irtija**, **E.D. Banks**, L.A. Porter

CHED **844.** Sustainability in the laboratory: Assessing green chemistry integration in the general chemistry curriculum. **M.C. Rivas**, L. Armstrong, G. Kerstiens, M.T. Robak, M.C. Douskey, A.M. Baranger

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Computational Chemistry

Cosponsored by COMP and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **845.** Generation of new liver X receptor ligands using state-of-the-art computational methods. M. Ndukwe, **K. Riley**

CHED **846.** Computational studies of formaldehyde reactions with HCN, ammonia, and pyrrole relevant to prebiotic chemistry. K. Thrush, **H. Loli**, J. Kua

CHED **847.** Characterization of the structure of vinyl cations. **C. Lodder**, B.N. Norris

CHED **848.** Impact of DNA strand length on duplex stability in solution and in a microarray environment via molecular simulation. **B. Rivard**, S. Cooper, L. Pelletier, J.M. Stubbs

CHED **849.** Searching for a Möbius conformation of cyclometaphenylene. **S. Cho**, S.M. Bachrach

CHED **850.** Nitrogen-substituted bisaryl dienes in the Diels-Alder reaction. **Z. Zayat**, S.M. Bachrach

CHED **851.** α-Conotoxins peptide mutants as Parkinson's therapeutics: A molecular dynamics study. **S. Walker**, O.M. McDougal, M. King

CHED **852.** Energy landscape of unsubstituted seven-membered ring oxocarbenium ion. **E. Castele**, K.A. Woerpel, J.D. Evanseck

CHED **853.** Theoretical energy determination of hydroxy-peroxy radicals derived from α-terpeniol using *Ab initio* and density functional theory calculations. **A. Alejandro**, C. Wilson, S. Drake, K. Dowda, R.S. Dabell, J.C. Hansen

CHED **854.** Temporary anion states in the field of permanent dipole and quadrupole moments. **D.C. Hiener**, M.C. Fair, M.F. Falcetta

CHED **855.** Conventional strain energies of the oxaphosphetanes and the oxadiphosphetanes. **B. Nash**, A. Smyly, D.H. Magers, S.A. Smith

CHED **856.** Investigation of hyroxy-peroxy radicals derived from *R-limonene: A theoretical approach*. **C. Calderon**, A. Alejandro, M. Dick, T. Murphy, M. Synelnikov, M. Russon, R.S. Dabell, J.C. Hansen

CHED **857.** Conventional strain energy in ketene acetals and ketene aminals. **S.G. Travis**, S.A. Smith, D.H. Magers

CHED **858.** Precision-biased statistical coupling analysis for use in rational protein design. **O. Chapman**, A.M. Leconte, A. Cavalcanti

CHED **859.** Molecular simulations reveal the importance of disulfide bridging in PrgW, a putative redox switch for plasmid replication. **S. Dornblaser**, B. Buttaro, V.A. Voelz

CHED **860.** Using electronics and sterics to affect the cyclization of angularly benzannelated enediynes. **T. Keel**, M.H. Daly, B.F. Gherman, J.D. Spence

CHED **861.** Computational investigation of isoquinoline alkaloids and scaffold replaced derivatives as LXR modulators. **D.A. Spadoni**, **C. Todd**, F. Payton-Stewart

CHED **862.** Propagation of hyperbolic secant wave packets: Visualizing the quantum momentum and potential field with numerical analytic continuation. **W. Garrett**, C. Lechak, B.A. Rowland

CHED **863.** Theoretical study of aerosol seeding via homoassociation of methane sulfonic acid. **C.M. Kottke**, H.K. Hernandez-Soto

CHED **864.** Computational characterization of the form of Ag(phen) for amination and azirdination reactions. **P.M. Birschbach**, J. Scanlon

CHED **865.** Structure-based prediction of small molecule modulators of DNMT3A. **Y. Markov**, A. Schlessinger

CHED **866.** Theoretical study of ligand effects on homogeneous hydrogenation catalyzed by iron-pyridone complexes. **E.F. Curl**, L. Boisvert, T.V. Harris

CHED **867.** Mathematical model for copper homeostasis in *Pseudomonas aeruginosa*. **J.C. Roth**, B. Kozemzak, J. Parmar, P. Mendes

CHED **868.** Effect of ligand chemistry in mononuclear metal catalysts on the intramolecular features of the water oxidation mechanism. **K. Hunter**, J. Alvarado, E.A. Jarvis

CHED **869.** ONIOM model of malonate decarboxylation: Significance of the hydrogen bonding buckle. **L. Andreola**, I. Pathiraja, S.M. Firestine, A. Tamez, D.J. Fox, J.D. Evanseck

CHED **870.** Interaction energies of triclosan complexes: Effects of substituent groups. **A. Jimenez**, K.R. Jorgensen

CHED **871.** Effect of vacancy defects on ion transfer in carbon nanotubes. **B.A. Collins**, T.D. Shepherd

CHED **872.** Coarse-grain simulations of confined water within carbon nanotube systems. **J. Chisholm**, T.D. Shepherd

CHED **873.** Is a planar $C_{16}N_{12}$ possible? **M. Alsarraj**, M. Vaziri, J. Song

CHED **874.** Inductive and hyperconjugative effects on carbocations. **J.J. Nysschen**, B.A. Modhera, E.D. Glendening

CHED **875.** Energetic and structural analysis of metallo-heterofullerene derivatives of C_{20}: $C_{19}M$ (M = 3d transition metals). **J. McDonald**, K.A. Beran

CHED **876.** TD-DFT potential energy surfaces and nonadiabatic dynamics of indole by surface hopping with Newton-X. **K.M. Vorwerk**, W. Kennerly

CHED **877.** Computational quantum chemistry studies of metal oxide clusters. **S. Partovi**, L.M. Thompson, H.P. Hratchian

CHED **878.** Thermodynamic properties of the loss of CH_3SH from protonated methionine. **D. Devore**, P.B. Armentrout, J. Johnston

CHED **879.** Withdrawn.

CHED **880.** Theoretical study of the formation of CH_3SO_3H from the reaction of CH_3SO_2H and OH radical. **W.L. Rebelsky**, H.K. Hernandez-Soto

CHED **881.** Computational study of CO adsorption on a platinum-modified faujasite zeolite. **K.A. Parrish**, **M.D. Fellows**, H.K. Hernandez-Soto

CHED **882.** Gas-phase transition states of proline tripeptides. **P. Arcoria**, J.C. Poutsma, V.H. Wysocki, A. Somogyi

CHED **883.** Influence of hyperconjugative and inductive effects on the acidities of carboxylic acids. **R.C. Rudisell**, E.D. Glendening

CHED **884.** Effects of basis set on the energy levels of highly charged ions. **J. Ortiz-Soto**, **J.I. Vega-Sánchez**, N.A. Lopez, J.A. Santana

CHED **885.** Theoretical investigation of N2C=CO2. V. Nguyen, **D. Corey**, J. Song

CHED **886.** Exploring metal surface catalytic effects on Li-S batteries with DFT calculations. **C.R. Bernard**, J.A. Santana

CHED **887.** Absorption and fluorescence of indole and tryptophan by TD-DFT. **J. Gerard**, W. Kennerly

CHED **888.** Density functional theory investigation of the interaction between acetone and chloroform. **M.E. Furgione**, R.J. Olsen

CHED **889.** Characterizing the Jahn-Teller effect in manganese trifluoride: A molecular modeling approach suitable for early undergraduate and AP high school chemistry students. **K.A. Shaikh**, S. Warrick, L. Gurung, D. Kwak, J.A. Bumpus

CHED **890.** Solvent effects in the dynamics on potentials with post-transition state valley ridge inflection points. **F. Malik**, Z.C. Kramer, B.K. Carpenter, G.S. Ezra, S. Farantos, S. Wiggins

CHED **891.** Computational study of the mechanistic effect of fluorine groups on the ring-opening polymerization of ε - caprolactone with Al-centered catalysts. **C. Ortiz**, A. Longo, J.M. Fritsch, B. Wilson

CHED **892.** Computational modeling of sodium laurate surfactant in the presence of aqueous divalent cations at the oil-water interface. **K.T. Chippindale**, K.E. Johnson

CHED **893.** Thermodynamics and SN2 mechanism of the loss of ammonia from protonated methionine. **A.A. Chen**, P.B. Armentrout, J. Johnston

CHED **894.** MR-MP energy levels of ions in the Li, Be and B isoelectronic sequences. **N.A. Lopez**, J.I. Vega Sánchez, J. Ortiz-Soto, J.A. Santana

CHED **895.** Using molecular dynamics simulations to investigate novel reaction events: A case study with iron carbonyls. **J. Liu**, L. Wang

CHED **896.** Investigation of micelle formation using molecular modeling and NMR. **C. Lewis**, F.H. Billiot, E. Billiot, K.F. Morris, Y. Fang

CHED **897.** Computational investigations of aldol reactions of aromatic enolates and aldehydes. **A. Zolfaghari**, N.M. Wachter, S. Mazumder

CHED **898.** Elucidation of electrochromic materials utilizing TDDFT. A.L. Tomlinson, **A.R. Green**

CHED **899.** Computational studies of oxygen bond lengthening with group-10 metal clusters. **D. Gray**, M. Paul

CHED **900.** Withdrawn.

CHED **901.** Parameter development for pseudouridine. **A. Ustoyev**, M.C. Nagan

CHED **902.** Molecular modeling studies on the realkylation of Aged-Acetylcholinesterase (AChE) by Quinone Methide Precursors (QMPs). **R. Hopper**, I. Pelfrey, R. McCauslin, R.J. Yoder

CHED **903.** DFT analysis of various porpholactone isomers. **R.F. Lalisse**, M. Guberman-Pfeffer, J. Gascon, C. Bruckner

CHED **904.** Protein-ligand docking with HADDOCK: The effects of input protein conformational differences on the success of docking. **K.R. Reinke**, J. Grinstead, A. Bonvin

CHED **905.** Substitution group effect on the inhibition of ubiquitin C-terminal hydrolases for Parkinson's disease study: Synthesis and computational analysis. **M. Liang**, D. Xiao

CHED **906.** Utilization of molecular dynamics to examine the physical properties of hydrocarbon mixtures from 293-373 K. **J. Winkler**, T. Knippenberg

Section I

Moscone Center

Hall D

Undergraduate Research Posters

Environmental Chemistry

Cosponsored by ENVR and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **907.** Correlation study between particulate matter and PAH concentrations through the bio-monitoring of pine tree leaves. **R. Moran**, **S. Cortez**, S. Deprele

CHED **908.** Differential impact of chitin and chitosan on heavy metal pollution in water samples. **J. Caldwell**, J. Mendez

CHED **909.** Continued investigation of the mechanism of biosorption of lead. **T. Robertson**, D.J. Schauer

CHED **910.** Atmospheric applications of deliquescence relative humidity determined by quartz crystal microbalance. **A.C. Burrows**, H. Holst, C.M. Strollo

CHED **911.** Impact of the position of the chloro-substituent in chloroformate reactivity. **J. Wirick**, M.J. D'Souza

CHED **912.** Withdrawn.

CHED **913.** Changes to As, Cu, Fe, Mn and Zn concentrations in soil resulting from the application of poultry manure. R.D. Foust, **K. Hull**

CHED **914.** Soil analysis for the greater Albion Community Garden Network. **R. Ford**, K.M. Metz

CHED **915.** Assessment of heavy metals in subsistence-harvested alaskan pinniped vibrissae. **C. Gotluru**, **T. Juneja**, P. Ferdinando, K. Cash, K. Sekou, A. Hirons, **D.G. Giarikos**

CHED **916.** Laboratory simulation of the open limestone channel at abandoned mine: Swank 13. **J.M. Schulte**, P. Youmbi, D. Madl, R. Krupa, J.Z. Bandstra, E.P. Zovinka

CHED **917.** Study on the synthesis of ADA chelating cellulose and its adsorptive capability. **L. Yi**, S. Wenjian, P. Yang, J. Fangyuan, L. Xiaoxiao

CHED **918.** Inventory platform manages chemical risks, addresses chemical accountability, and measures cost-effectiveness. **L. Neff**, K. Roeske, M.J. D'Souza

CHED **919.** Singlet oxygenation of Lipitor and Lescol. **G.D. Tejeda**, K.E. O'Shea

CHED **920.** Factors controlling the regioselectivity and rate of arene bromination by aqueous BrCl and related brominating agents: Influence of steric effects. **K.R. Martin-Culet**, J.D. Sivey

CHED **921.** Investigating lead sources near a secondary lead smelting site: Using antimony as a pathfinder element. **D. DeWilde**, **K. Ryncarz**, **N. Aist**, M. Ketterer, S. Youtsey

CHED **922.** Examination of the composition of the lipid component of natural organic matter using ultrafiltration with organic solvents and NMR analysis. **A. Kub**, J. Rice

CHED **923.** Distinguishing between dissolved reactive phosphate and bioavailable phosphate for the development of a biophosphate sensor. **A. Cooper**, E. White, C. Lemus, H. Goodson

CHED **924.** Photocatalytic degradation of tetracycline using floating PMMA-TiO_2 macrospheres. **A.C. Hartley**, J.D. Glover, J.E. Boyd

CHED **925.** Assessment of hydroxyl radicals production during ultrasonic irradiation for potential treatment of diphenhydramine pollution. **J.M. Rosado**, D. Cui, K.E. O'Shea

CHED **926.** Photochemical degradation of oil in seawater. **D. Chang**, S. Hok, T. Bui, A. Lam, M. Eclevia, W.J. De Bruyn, C.D. Clark

CHED **927.** Using 3-component hydrocarbon mixtures to model the properties of catalytic hydrothermal conversion fuels. **S.Y. Ye**, M. McLaughlin, D.J. Luning Prak

CHED **928.** Ozone in Sequoia National Park: Linking ozone production in the San Joaquin Valley to trends in vegetative impacts in Sequoia National Park from 2000-2016. **C. Buysse**, S. Pusede, A. Kotsakis

CHED **929.** Effects of anthropogenic activities on the water quality of the Huron River and its contributing streams. J. Vites, **O. Hajihassani**

CHED **930.** Withdrawn.

CHED **931.** Groundwater pollution reduction through biochar adsorption of herbicide Dacthal. **O.O. Harrison**, E. Baker, S.K. Saha, A. Saha

CHED **932.** Modeling the kinetics of trace metal ion speciation: The influence of calcium ion on disjunctive ligand exchange. **L. Rea**, N.E. Boland

CHED **933.** Human effect on potentially toxic metal concentrations in the soils of Scotland. **K. McCarthy**, C. Davidson

CHED **934.** Viability of fecal coliform bacteria in beach sand and lake sediments. **C.M. McManus**, D.S. Karpovich, J.L. McEvoy

CHED **935.** Determination of the mechanism for trihalomethanes and nicotinamide in basic medium for a water disinfection device. M. Dorko, **S. Espy**

CHED **936.** Effect of silver nanoparticles with varying capping agents on the growth of kale (brassica oleracea). **A. Agloro**, A.L. Smalley

CHED **937.** Fate and toxicity of BPA in two native plants, blue bush lake beans (*Phaseolus vulgaris)* and switchgrass *(Panicum virgatum),* to explore their phytoremediation potential. **J.C. Murphy**, A.K. Merrill, P. Das

CHED **938.** Phase transitions of biologically-derived components in sea spray aerosols and investigation into the chemical complexity of aged SSA. **M. Alves**, A. Estillore, J. Trueblood, V.H. Grassian

CHED **939.** Quantification of 11-nor-9-carboxy-tetrahydrocannabinol in wastewater from Washington State to estimate consumption patterns of cannabis use. **A. LaRock**, J. Sadetsky, D. Westerman, D.A. Burgard

CHED **940.** Quantification of THC-COOH to estimate cannabis consumption trends via wastewater based drug epidemiology. **J. Sadetsky**, A. LaRock, R. Carpenter, D.A. Burgard

CHED **941.** Urban and rural land use contributions to phosphorus and E. coli pollution: A case study on Bad Axe Creek. **M. Dobulis**, E.M. Greeson, K.L. Kwiatkowski, T. Benedict, O. Bishop, A. Yankley, K. Underwood, C.M. McManus, T. Sivy, D.S. Karpovich

CHED **942.** Synthesis of amino acids coupled to 2,6-pyridine dicarboxylic acid, and evaluation of their affinity towards metals. **E. Luta**, **A. Stedman,** S.G. Tajc

CHED **943.** Graphene-doped polyethylene electrodes used to produce hydroxyl radicals for water purification. **A. Wallace**, L. Slaymaker, R.J. Hamers

CHED **944.** Characterizing heavy metal sequestration in a bioswale at Pomona College. **Z. Evans**, H. Van Ryswyk, M. Los Huertos

CHED **945.** Analyzing the atmosphere of crystal cave: Understanding sources and sinks of trace gases. **A.W. Jarnot**, S. Hughes, D.R. Blake

CHED **946.** Environmental drivers of cyanobacterial blooms and toxin production in Lake Winnebago, Wisconsin. **A. Tomczyk**, S.L. Bartlett, R.M. Kutzner, J. Piatt, T.R. Miller

CHED **947.** Algal toxin dynamics and environmental indicators in Green Bay, Wisconsin. **R. Kutzner**, S.L. Bartlett, A. Tomczyk, J. Piatt, T.R. Miller

CHED **948.** Estimation of the source of atmospheric inputs of selected metals and metalloids to the Pacific northwest (USA). **M. Sousa**, C. Welty, D. Price, M. Cummings, F.M. Dunnivant

CHED **949.** Absorption and translocation of lead (II) Nitrate within *Coriandrum sativum*. **J. Wilson**, D.J. Schauer

CHED **950.** Chemistry of imidazole forming reactions and reactive uptake of hydrocarbons. **A. Sager**, J.M. Ackendorf, M. Galloway

CHED **951.** Photolysis of the suburban-use herbicide trifluralin on retail mulch surfaces. **M. Kaur**, F. Pavlovici, K.J. Bisceglia

CHED **952.** Gadolinium complexes for catch-and-release of phosphates. **C. Zeller**, K. Peterson, S. Harris, V.C. Pierre

CHED **953.** Synthesis of water-stable material-organic framework at room temperature. **N. Le**, K.T. Jackson, D. Eseonu, F. Mensah

CHED **954.** Effect of substrate on the growth of *Manilkara bidentata* at Finca Nolla Camuy, Puerto Rico: Applications in environmental chemistry. **F.A. Portero Camacho**, **K.R. Reyes Sanchez**, R.J. Mayer Arzuaga

‡ *Cooperative Cosponsorship*

CHED **955.** Total conversion of mixed algae lipids to biofuels over heterogeneous catalysts. **E. Timmel**, D.S. Heroux

CHED **956.** Kinetic studies of the photolysis of dicarbonyls. **M. Ryan**, C.M. Strollo

CHED **957.** Optimization of a cellular phone-based method for nitrate/nitrite detection using paper-based fluidic devices. **K.L. Kwiatkowski**, Z. Velasco, K. Cissell

CHED **958.** Withdrawn.

CHED **959.** Determining metal content in abandoned mine soils. **C. Lupse**, K. Brotherton, J.D. Leyba

CHED **960.** Investigation of 3,4-Methylenedioxymethampthetamine (MDMA) in Minnesota's natural waters by headspace solid-phase microextraction (HS-SPME) GC-MS. **M. Hanson**, N.R. Lien

CHED **961.** Caffeine and its metabolites as biomarkers: Analyzing caffeine, theobromine, and theophylline concentrations in wastewater discharge of the Winona, MN area waters and the development of greener analytical techniques. **A. Paulson**, J.L. Franz

CHED **962.** Quantification of levoglucosan in $PM_{2.5}$ atmospheric aerosols using GC/MS: Seasonality of a biomass burning tracer in Central Arkansas. **J. Gann**, **A. Gatmaitan**, J. Higgins, D. Hughes, C.D. Hatch

CHED **963.** Selective quantification of chlorine and bromine in water using halogen trapping agents. **R.P. Dias**, N.A. Race, J.D. Sivey

CHED **964.** Measurement of multicomponent aerosol optical properties using pulsed laser cavity ring-down spectroscopy. **H.E. Kay**, **A.N. Jarman**, J. DeYoung, J.A. Land, K.S. Dooley

CHED **965.** Effect of ozonization on the potential toxicity of biochar. A. Pullin, O. Sacko, **J.W. Lee**

CHED **966.** Spatial determination of organic matter on sediment particles by scanning electron microscope analysis. **M.M. Clay**, F.M. Dunnivant

CHED **967.** Heavy metal analysis of fish inhabiting varying light depth zones of the ocean. **M. Sousa**, C. Welty, F.M. Dunnivant

CHED **968.** Dissolution of uranyl silicate minerals in uranyl peroxide nanocluster forming environments. **C.J. Parker**, H.L. Lobeck, E. Balboni, P.C. Burns

CHED **969.** Formation of unanticipated ring cleavage products during $OH^{\bullet}$ and $SO_4^{\bullet-}$ water treatment. **B. Skeel**, J. Van Buren, C. Prasse, D.L. Sedlak

CHED **970.** Determination of metal concentrations in sediments of Big Walnut Creek. **H. Quinn**, J.M. Esson, M. Hoggarth, K. Svitana, K. Lathrop, N. Hess

CHED **971.** Novel compounds extracted from endophytes of *Bassia Scoparia*. **K. Hardy**, M.D. Halling

CHED **972.** Multi-Regression factors influencing textile dye adsorption on activated carbon. **S. Aanonsen**, P.A. Snetsinger, E. Alkhatib, A. Alanazi

CHED **973.** Traces of chemical compounds in Carraízo Reservoir and Sergio Cuevas Water Treatment Plant in Puerto Rico. **N.M. Casellas-Cruzado**, G. Infante-Méndez

CHED **974.** Studies on the organic matter in soils along a hypersaline lagoon. A. Colon Santiago, D. Soto Bonilla, **W. Colon Colon**, J.I. Ramirez Domenech

CHED **975.** Enhancement of atmospheric nucleation by ion pairs. **M.A. Olson**, J. Schlecht, S. Pavlenko, S.J. Keasler

CHED **976.** Fat from the Green iguana (*Iguana iguana)* as potential source of lipids for production of biodiesel. **L. Renta Morales**, L. Romero, L. Torres

CHED **977.** Investigating the structure of humic acid using a molecular probe. **C. Zdunich**, J. LaFontaine, G. Chilom

CHED **978.** Effect of humic acid treatment on the removal of methylene blue from aqueous solution. **R. Wolsleger**, O. Ruiz, G. Chilom

CHED **979.** Novel compounds extracted from endophytes isolated from *Juniperus osteosperma*. **S.A. Ellsworth**, M.D. Halling

CHED **980.** Chemical and optical properties of model brown carbon systems characterized by UV/visible spectroscopy and aerosol mass spectrometry. **H. Welsh**, M. Alexander, L. Hawkins

CHED **981.** Natural homemade teeth whitening: A comparison of natural and commercial products. **M. Nafea**, **M. Tomaraei**, P.J. Iles, L.D. Giddings, R.V. Valcarce, N.R. Bastian, M. Alvarez, R. Holcomb

CHED **982.** Investigating the effects of copper-based nanoparticles/compounds in zucchini (*Cucurbita pepo)*. **M. Hernandez Molina**, C. Tamez, J.A. Hernandez, J. Peralta, J.L. Gardea-Torresdey

CHED **983.** Heavy metal indication through colored complexes and its biosorption implications. **M.R. Reeves**, D.J. Schauer

CHED **984.** Relationship between pH and the extent of hydration of atmospheric photosensitizers. **M. Ippolito**, M. Galloway

CHED **985.** Comparison of organophosphate pesticide presence in honey using QuEChERS and gas chromatography mass spectrocopy. **C. Westgate**, S.A. Waratuke

CHED **986.** Environmental photochemistry of the polycyclic musks tonalide and galaxolide. **B.G. Anderson**, S.W. Beck, C.J. Heiling, D. Martinovic-Weigelt, K.H. Wammer

CHED **987.** Environmental photochemistry of dienogest: Photolysis, regeneration, and product bioactivity. **M.K. Hankard**, S.M. Berg, N.C. Pflug, D.M. Cwiertny, D. Martinovic-Weigelt, K.H. Wammer

CHED **988.** Aqueous photolysis of the steroid gestrinone in the presence of sodium azide. **J. O'Brien**, S.M. Berg, N.C. Pflug, D.M. Cwiertny, K.H. Wammer

CHED **989.** Abandoned heavy metal mine releases to the Middle Fork of the Salmon River. **D. Price**, M. Sousa, C. Welty, F.M. Dunnivant

CHED **990.** Phytoremediation potential of switchgrass (*Panicum virgatum)* a native plant, to clean-up Bisphenol-A (BPA) contaminated aquatic systems. **A.K. Merrill**, J.C. Murphy, P. Das

CHED **991.** Synthesis of platinum(II) water soluble luminescent dye for sensing. **J. Oh**, J.E. McGarrah

CHED **992.** Survey of radiogenic metals in Salt Lake County, Utah. **B. Mower**, P.J. Iles, L.D. Giddings, R.V. Valcarce, N.R. Bastian, M. Alvarez, R. Holcomb

CHED **993.** Analysis of drinking water samples for perfluorooctanoic acid and 1,2,3,-trichloropropane by LC-MS in the Clovis metropolitan area. **B. Flynn**, **D. Fujino**, J. Ghuman, **K. Johnson**, **J. Krauthammer**, D. Dormedy

CHED **994.** Electronic cigarette solution and vapor analysis with GC-MS and LC-MS. **M. Lazernik**, **P. Cole**, **M. Jones**, B. Shamp, D. Dormedy

CHED **995.** Evaluation of pectin as a target for biosorption of heavy metals. **M. Zerbe**, D.J. Schauer

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Geochemistry

Cosponsored by GEOC and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **996.** Water adsorption on goethite: CCN activation from Frenkel, Halsey and Hill activation theory. **R. Tumminello**, R. Meredith, C.D. Hatch

CHED **997.** Nitrate reduction in prebiotic chemistry. **V. Aguirre**, S. Churchman, M.M. Baum, D. VanderVelde, L.M. Barge

CHED **998.** Water adsorption on montmorillonite: Comparison of washed and unwashed clays. **M. Cassingham**, R. Tumminello, J. Kim, C.D. Hatch

CHED **999.** Modeled impacts of sulfuric acid leaching solution on two groundwater types in the Upper Cienega Creek Watershed. **C. Morel**, R. Tucci, J. Mcintosh

CHED **1000.** Sulfide-induced abiotic methylmercury transformation. **C. Kanzler**, A. Graham

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Green Chemistry & Sustainability

Cosponsored by CEI and SOCED

Financially supported by IEC Green Chem; Green Chemistry Institute

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1001.** Obtaining electricity from solar energy utilizing household products. **D. Romero**, **E. Zuniga**, E. Stemp, A. Calderon

CHED **1002.** Oxidative dimerization of 1-(2-thienyl)-pyrene. **L.M. Rhoda**, J.G. Rowley

CHED **1003.** Green synthesis of novel analogues of resveratrol: Toward unlocking new treatments for degenerative diseases. **E. Barth**, L. Daley, S.P. George, D. Paull

CHED **1004.** Pressure controlled continuous flow reactor synthesis of amides from aniline derivatives. **M. Turk**, M.T. Wentzel

CHED **1005.** Microwave synthesis and functionalization of vinylogous imines. **B. Lanigan**, A. Delawder, M. Manpadi

CHED **1006.** Green microwave nitration as an undergraduate organic chemistry lab procedure. **M. Nauman**, I.J. Levy

CHED **1007.** Towards green multistep synthesis in the Organic Chemistry laboratory curriculum: Conversion of alcohols to ketones via conventional heating. **L.T. Walsh**, I.J. Levy

CHED **1008.** Coffee grounds to ethanol: Green chemistry in the undergraduate lab. **D. Schultz**, A.E. Fischer

CHED **1009.** Application of natural fiber welding for the generation of novel horse hair composite structures. **M.C. Scully**, A.G. Burn, P.J. Fahey, D.P. Durkin, F. Vollrath, H.C. De Long, P.C. Trulove

CHED **1010.** Empirical model of Polymer Electrolyte Membrane Fuel Cells (PEMFC) using vulcan/Pt/Ce(III) catalysts in ethanol. **L. Lotti Diaz**, Y. Garcia Herrera, R. Guzman Blas

CHED **1011.** Development of a greener synthesis of diarylisoxazoles. **B. Leon**, **K. McCord**, N. Aoki, M. Bell, E. Petillo, L. Bastin

CHED **1012.** Greening the synthesis of virstatin: Finding an alternative solvent to dimethyl formamide. **M.T. McCauley**, K.A. Daus

CHED **1013.** Mechanochemical oxidation leading to porphyrins. **S. Everett-Hannah**, T.D. Hamilton

CHED **1014.** Withdrawn.

CHED **1015.** Synthesis of room temperature ionic liquids. **O. Alquzah**, T.R. Hayden

CHED **1016.** Flipping pre-labs for organic chemistry. **T. Edwards**, T.R. Hayden

CHED **1017.** Improving efficiency in the synthesis of oxindole-3-acetic acid: A key intermediate in the synthesis of 3-bromooxindole-3-acetic acid. **N. Ivanowsky**, E.J. Brush

CHED **1018.** Green dissolution techniques for the analysis of lead, arsenic, and cadmium in contaminated soils. **J. Andrews**, J.D. Leyba

CHED **1019.** Withdrawn.

CHED **1020.** Synthesis of camphor using ionic liquids. F.C. Mayville, **B.N. Gillott**, **K.M. Cappuccino**, **B.A. Dierolf**

CHED **1021.** Influence of water in preparation of metal-organic frameworks. **E.A. Morley**, D.J. Strong, J.D. Heglund, D.A. Mellinger, J.J. Pak

CHED **1022.** 3D Printing dye-sensitized solar cells. **P. Kurriss**, J. Loebelenz, J.C. Warner

CHED **1023.** Fischer esterification using solar irradiation. **C.R. Buckner**, D.J. Swartling

CHED **1024.** Thermal stability of white turnip peroxidase in the presence of calcium chloride and ethylene glycol. **C. Munson**, A. Hoffman

CHED **1025.** Investigating the breakdown of cellulosic materials in environmentally benign conditions. **C.L. Boyd**, **A.A. Talorico**, J.K. Berch

CHED **1026.** Ionic liquids as green extractants of biofuels. **J. Melessa**, **A. Everett**, D. Stapleton, A. Young, D. Thomas, R. Wolsleger, D. Warner, A.T. Koppisch, R.E. Del Sesto

CHED **1027.** Recycling AgCl waste into $AgNO_3$. **S. Max**, J. Esbenshade

CHED **1028.** Surfactants with reversible linkers for micelle-facilitated organic synthesis. **J.G. Haggett**, K. Craig, L. Krings, H. Martin, D. Brownholland

CHED **1029.** Synthesis of a proline-surfactant conjugate for stereoselective micelle-catalyzed organic reactions. **A.J. Szczodrowski**, D. Brownholland

CHED **1030.** Solventless Wittig reaction. **P. Liang**, W. Liang, S. Xie

CHED **1031.** Green modifications to the Hajos pathway to an important steroid intermediate. **C.H. Cooper**, J.K. Berch

CHED **1032.** Low toxicity extraction solvents for recovery of precious materials and environmental contaminants. **G. Ifijeh**, **C. Nwokolo**, R.E. Del Sesto

CHED **1033.** Dehydration of alcohols by solar irradiation. **S.M. Amin**, D.J. Swartling

CHED **1034.** Mechanochemical synthesis of porphine and bis-pocket porphyrin. **D. Cordero**, T.D. Hamilton

CHED **1035.** Room temperature ionic liquids as a green alternative for the extraction of acetaminophen. **V. Harris**, T. Hayden

CHED **1036.** Thermal decomposition pathways of guaiacol and 4-methylguaiacol under fast pyrolysis and gasification conditions. **A. Nguyen**, **C. Luong**, **E.B. Ledesma**

CHED **1037.** Evaluating replacement anti-freeze additives for use in silicone fluid mixtures: Low temperature behavior of isolated and bulk water species. **C.E. Miller**, T.M. Alam

CHED **1038.** Synthesis and investigation of the bactericidal properties of quaternary ammonium chloride monomers for thin-film copolymer coatings. **M. Jung**, C.L. Horgan, K. Hixon, N.E. Lee, S. Walker, R.W. Gurney

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Inorganic Chemistry

Cosponsored by INOR and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1039.** Size and shape analysis of inorganic materials for solar energy conversion. **S. Mackley**, F.E. Osterloh

CHED **1040.** Preparation and characterization of an iron oxide nanoparticle-bound copper(II) cyclam complex for phosphate ester hydrolysis. **M. Cruz Reyes**, B.R. Bodsgard

CHED **1041.** Coordination chemistry of verdazyl polypyridyl analogs: Monometallic systems and self assembled grids. D.J. Brook, **S. Shtargot**, C. Fleming, **G. Wantaniyakul**, B. Ploof

CHED **1042.** Potential green catalyst for the bleaching of cotton. **D. Abraham**, J.H. Davis

CHED **1043.** Tetra-substituted porphyrin with exo-dentate binding groups: Toward catalytic metalloporphyrin assemblies. **N. Maxi**, T.D. Hamilton

CHED **1044.** Comparison of commercial zeolite 4a and zif-95 on separation of methane from carbon dioxide and nitrogen. **M. Yang**, F. Tian

CHED **1045.** Investigation of HKUST-1 and related composites with protein adsorption. **R. Rupasinghe**, Z. Mensinger

CHED **1046.** Synthesis of imidazole, triazole, and benzimidazole salts. **S. Steger**, M.A. Guino-o

CHED **1047.** Dilithium (citrate) crystals and their relatives. **A. Cigler**, J. Kaduk

CHED **1048.** Synthesis and spectroscopic investigation of substituted salen and phthalocyanine chelating ligands. **O. Staples**, D. Perales, F.A. Fasulo, K. Wyss, J.M. Sears, T.J. Boyle, R.A. Kemp

CHED **1049.** Probing the interaction of vanadate with alcohols and amines via ^{51}V-NMR spectroscopy: An inorganic laboratory exercise. **M.E. Donaldson**, **A. Taylor**, C.M. Davis

CHED **1050.** Synthesis of a seven coordinate catalyst for bleaching. **R. Guthrie**, J.H. Davis

CHED **1051.** Continuing catalytic studies for the production of cyclic organic molecules using $[(C_6F_5)C_5H_4]Co(CO)_2$ as a catalyst. **O.P. Fry**, E. Hawrelak

CHED **1052.** Withdrawn.

CHED **1053.** Optimization of the crystallization of aluminum oxometallic clusters. **M. Cole**, E. Eitrheim, T. Forbes

CHED **1054.** Synthesis and NMR characterization of a new series of thiazole-2-carboxaldehyde thiosemicarbazone ligands and their Pd(II) complexes. **K.L. Lawson**, E.C. Lisic

CHED **1055.** Speciation of mixed metal hydroxo-aquo aluminum clusters. **A. Samuel**, B. Fulton, D.W. Johnson, A.F. Oliveri, C. Colla, C.K. Perkins

CHED **1056.** Fabrication and analysis of a photovoltaic cell with a bismuth vanadate photo-anode and potassium iron(III) hexacyanoferrate(II) cathode. **J. Denney**, K.E. Peterman

CHED **1057.** New series of tungsten aryloxide pyridine complexes that exhibit contact shifted paramagnetic 1H NMRs. **J. Herder**, T. Graybill, M. Genzink, C. Kriley, G.J. Balaich

CHED **1058.** Synthesis and NMR characterization of a new ligand, 2-acetylpyrazine-tert-butylthiosemicarbazone, and its palladium (II) complex, [Pd(APZ-tBTSC)Cl]. **S. Grossarth**, A.R. Nesbitt, E.C. Lisic

CHED **1059.** Synthesis, characterization, and unusual solvation and luminescent properties of terbium amine complexes. **L.A. Ligon**, J.J. Stace

CHED **1060.** Exploring the coordination chemistry of a bulky succinimide ligand. **C. Martin**, **X. Xhani**, G.J. McManus

CHED **1061.** Synthesis and characterization of tris(4,4-dichloro-2,2-bipyridine) ruthenium (II). **J. Bence**, D.G. Giarikos

CHED **1062.** Direct observation of ion pairing in aqueous solutions of lithium carbonate. **L. Fredenburg**, J.C. Goeltz

CHED **1063.** Synthesis and reactivity of bromofumaronitrile (1-bromo-1,2-dicyanoethylene): Useful synthon for dicyanoacetylene. **J. Lois**, J.P. Fitzgerald

CHED **1064.** Coordination chemistry of group 12 thiocyanate complexes containing bicyclic isothioureas. **E. Rojas**, P.M. Secondo

CHED **1065.** Synthesis and characterization of a series of tris(3-phenylpyrazolyl)borato zinc(II) oxocyclohexadienolate complexes derived from *in situ* oxidation of parent catecholate complexes. **D. Isaacs**, M. Bezpalko, N.A. Piro, W.S. Kassel, W.G. Dougherty

CHED **1066.** 5-acetyl-imidazol-2-ylidene-4-olate ligand (IMes-acac): Synthesis, coordination chemistry and evaluation of the electronic communication. **S. DePeter**, V. Mallardo, A. Nano, G. Dahm, N. Lugan, S. Bellemin-Laponnaz, V. César

CHED **1067.** Synthesis and application of copper metal-organic framework for naked eye, colorimetric detection of toxic organic molecules. **K. Curtin**, J.K. Vohs

CHED **1068.** Synthesis, characterization and electrochemistry of a ruthenium nitrosyl carbon-bound diazeniumdiolate porphyrin complex. N. Xu, **A. Bevak**, **B. Armstrong**, E.G. Abucayon, G.B. Richter-Addo

CHED **1069.** Temperature dependence of solution processed formamidinium iodide based perovskite thin films. M.C. So, **C. Hutcherson**

CHED **1070.** Green chemistry catalysts for transfer hydrogenation reactions. **K. Idrees**, E. Rajaseelan

CHED **1071.** Computational and experimental studies of methyltrioxorhenium catalyzed olefin hydrogenation. **K. Idrees**, N. Lambic, E.A. Ison

CHED **1072.** Effects of solvent treatment on morphology of Methylammonium Lead Iodide (MAPbI3) perovskite thin films. **V. Cherrette**, M.C. So

CHED **1073.** Synthesis and characterization of rhodium(III) complexes using mixed polypyridyl ligands. **P. Nunez**, D. Amarante

CHED **1074.** Synthesis of tin phosphide and tin nanomaterials. **C. Stevens**, B.A. Hernandez-Sanchez, R.A. Kemp, D.A. Dickie, T.N. Lambert

CHED **1075.** Importance of the zinc metal center and thione/selone antioxidant properties. **A.M. Owen**, J.M. Murphy, B. Stadelman, J.L. Brumaghim

CHED **1076.** Synthesis and reactivity studies of rhodium complexes supported by a PNSi pincer ligand. **B. Morse**, C.J. Pell, O. Ozerov

CHED **1077.** Development of a solid state educational lab. **M.M. Scanlan**, B.J. Bellott

CHED **1078.** Synthetic and structural studies of low-melting ionic materials with carborane cluster anions. **M. Raymond**, **A.R. Talosig**, A.S. Svetlanova-Larsen

CHED **1079.** Electrocatalytic reduction of CO_2 by $[Pd(dpk)Cl_4]$ and $[Pd(dpk)_2Cl_2]^{+2}$. **R. Higgins**, R.M. Granger

CHED **1080.** Catalytic activity of 1,3-bis(2-pyridyl)imidazolin-2-ylidene supported metal complexes. **R. Cerbone**, R.J. Swails

CHED **1081.** Coordination chemistry of group 12 thiocyanate complexes containing benzimidazole and its anionic analog. **T. Lyons**, P.M. Secondo

CHED **1082.** Structure and activity of complexes supported by neutral and cationic N-heterocyclic carbene ligands. **S. Kariofillis**, R.J. Swails

CHED **1083.** Imidazole for pyridine: Its influence on the coordination of nickel(II) aromatic oxime complexes. **A.A. Ibarra**, M.J. Prushan

CHED **1084.** Applications of duplex pincer chemistry. **K. Motley**, J. Lohrman, K. Bowman-James

CHED **1085.** Polynuclear inorganic and organometallic complexes of ruthenium and their biological activity. F.A. Beckford, **M. Niece**

CHED **1086.** Palladium complexes of multidentate resorcinarene surfactants. **A. Benedict**, A.V. Skinner, B. Ramjee

CHED **1087.** Microwave assisted syntheses of CB_{11}^- carborane derivatives. **A.B. Shaff**, M.A. Juhasz

CHED **1088.** Discoveries in the antimicrobial properties of ZnO plate and rod morphologies. **A. Schnoebelen**, A.T. Bloemer, B. Torrance, P. Window, W.L. Cody, E. Steinmiller

CHED **1089.** Synthesis of ligands from the amides of 2,6-pyridinedicarboxylic acid. **H. Sturm**, J. Feder, J. Bodwin

CHED **1090.** Preparation and reactivity of platinum(II) complexes with dipropylenetriamine ligands. **A. Zahn**, K. Williams

CHED **1091.** Structural analysis of vanadium and peptide complexes. **A. Brechbill**, J.A. Dabrowski

CHED **1092.** Synthesis and characterization of novel fluoro-bridged copper(II) complexes. **B. Johnson**, L. Yang

CHED **1093.** Synthesis and characterization of copper(II) complexes supported by pyridylamide ligands. **G. Williams**, L. Yang

CHED **1094.** Switchable catalysis and related processes. **A. Laughlin**, J.L. Brosmer, P. Diaconescu

CHED **1095.** Simultaneous electrodeposition and recrystallization of silicon on gallium. **M. Cain**, G. LeBlanc

CHED **1096.** Systematic microwave-assisted synthesis of rhodium(I) and iridium(I) complexes with ambipolar polyimine ligands and the effect of the ligand's functional groups on their photophysical properties. **B. Hua**, G.A. Salazar-Garza, C.M. Williams, V. Nesterov, M.A. Omary

CHED **1097.** Solid state synthesis of copper sulfide using a NaCl-KCl flux. **S.A. Donnelly**, B.J. Bellott

CHED **1098.** Heterogeneous MOF built from heterotritopic linkers and infinite secondary building units. **M.B. Morla**, N.R. Catarineu, O.M. Yaghi

CHED **1099.** Electrocatalytic conversion of CO_2 using molecular manganese carbonyl based catalysts. **P.J. Smith**, M. Stanbury, E. Gouré, J. Compain, S. Chardon-Noblat

CHED **1100.** Peculiar properties of quantum dots: Cadmium sulfide/zinc sulfide nanoparticles. **K. Parson**

CHED **1101.** UMCM-1 protein adsorption and the effects of post-synthetic modifications of UMCM-1-NH_2 on protein adsorption properties. **A. Helmin**, Z. Mensinger

CHED **1102.** Dye sensitized solar cells: A push towards lowering cost and improving efficiency. **K.L. Digan**, C.A. Sweet, C.J. Timpson

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

CHED **1103.** Synthesis of monometallic nickel (II) halide complexes with secondary phosphines as building blocks for hydrogenase mimics. **A. Frantz**, N. Downes, T.W. Chapp

CHED **1104.** IR study of the particle-polymer interface in MOF mixed matrix membranes. **A.P. Odegard**, J.C. Moreton, S. Cohen, L.B. Benz

CHED **1105.** Microwave assisted metal nanoparticle synthesis. **L. Felix**, M.O. Montes

CHED **1106.** Cytotoxicity and uptake of platinum compounds in cancer cell lines. **H. Evie**, B. Duke, K. Williams, B.B. Williams

CHED **1107.** Synthesis and characterization of $[Rh(bopy)_2(dppz)]^{3+}$ and $[Rh(bopy)_2(phi)]^{3+}$ (bopy = 2-Benzoylpyridine): New potential metallointercalators supported by a mixed nitrogen/oxygen donor ligand. **M.R. Norton**, S.C. Haefner

CHED **1108.** Synthesis and characterization of some new iodobismuthates. **M. Barnhill**, L. Peterson

CHED **1109.** Synthesis of polymerizable phosphines from inexpensive starting materials. **H.K. Nguyen**, J.W. Gohdes

CHED **1110.** Synthesis of amido(thio) urea based rhenium (I) tricarbonyl complexes. **W. Evans**, M.O. Odago

CHED **1111.** Employing flexible ligands to construct metal-organic frameworks. **A.J. Soares**, G.J. McManus

CHED **1112.** Photophysics of cobalt-zirconium heterobimetallic materials with ancillary amine ligands. **M. Bedford**, N. Celia, A. Stone, A. Hill

CHED **1113.** Optimization of trivalent americium oxidation by sodium bismuthate. **N. Byrne**, P.I. Molina, K. Kozma, M.D. Nyman, L.M. Mascavage

CHED **1114.** Ruthenium polypyridyl complexes: Synthesis, spectroscopic characterization, and reactivity with CT-DNA. **J. Khuri**, H. Acquaye

CHED **1115.** Remarkably sensitive ^{13}C NMR approach to quantifying electronic characteristics of isocyanide ligands. **Z. Wood**, J.C. Applegate, N.R. Erickson, M.D. Hart, M.V. Barybin

CHED **1116.** Synthesis and coordination chemistry of new sterically hindered Schiff-base ligands. **M. Suchewski**, C.A. Bradley

CHED **1117.** Small molecule reactivity of Cp*Co(I) fragments. **A. Kayser**, C.A. Bradley

CHED **1118.** Development of a biomimetic hydrolysis catalyst consisting of a zinc containing molecular imprint polymer. **B. Doherty**, J.W. Gohdes

CHED **1119.** Palladium-catalyzed cross-coupling reactions: A clean synthetic method to assemble complex organic molecular frameworks. **P. Pham**, M. Young

CHED **1120.** Preparation of metal-organic frameworks containing N-heterocyclic carbene catalysts. **K. Campbell**, **B. Crabb**, T. Sarver, M. Shoukry, M.C. Perry, L.G. Beauvais

CHED **1121.** Developing materials for the purification of natural gas: Thermodynamic and kinetic studies of small molecule binding to iron phosphine complexes. **R. Gustafson**, J.W. Gohdes

CHED **1122.** Spin crossover and valence tautomerism in discrete and extended polymetallic systems. **A. Nguyen**, B. Ploof, D.J. Brook

CHED **1123.** Manganese(III) polymolybdate based single chain magnets. **B. McKenna**, S. Nellutla

CHED **1124.** Synthesis and characterization of silylated drug derivatives. **C.L. Burton**, D.L. Austin, K. Gwilt, W.W. Brennessel, B.M. Kraft

CHED **1125.** Systematic investigation into the bonding, electronic structure, and reactivity of metal/soft-donor biomimetic complexes. **H.C. Williams**, E. Hanna, J. Brown-McDonald

CHED **1126.** Withdrawn.

CHED **1127.** Investigation of group 13 bonding properties with bulky N-heterocylic carbenes following the synthesis and characterization of an imidazolium salt precursor. **D. Carone**, J.K. Vohs

CHED **1128.** Computational and experimental analysis of vandium (V) dipicolinate using ^{51}V NMR spectroscopy. **M. Feinman**, J.M. Fautch

CHED **1129.** Preparation of zeolitic materials from Western Pennsylvania coal fly ash. **A.M. Krol**, D.A. Polvani

CHED **1130.** Further investigation of transition-metal substituted polyoxotungstates in non-polar solvents using 2D DOSY P-31 NMR and density functional theory. **W.B. Swanson**, **J.R. Verdi**, M.M. Kozik

CHED **1131.** New multifunctional bis(amidine) ligands for highly luminescent coinage metal assemblies: Synthesis, structures, and coordination behavior. **A. Calderon**, O. Ugarte Trejo, N. Bhuvanesh, M. Stollenz

CHED **1132.** Investigation of antimicrobial properties of copper (II) ions in polyvinyl acetate. **K. Nelson**, J.M. Fautch

CHED **1133.** Energy-conserving inorganic pigments. **M.C. Bixby**, J.L. Hunting

CHED **1134.** Electron-rich organometallics: Featuring multiple isocyanoazulene ligands terminated with thiol anchoring groups. **K. Hicks**, M.V. Barybin

CHED **1135.** Molecular tweezers for catalytic hydrogenation and dehydrogenation. **T. Bader**, **B. Haslp**, G.M. Edvenson

CHED **1136.** Synthesis and x-ray crystal structure studies of dinitrosyl iron complexes based on 1, 10 - phenanthroline derivatives. **C.A. Koroni**, L. Li

CHED **1137.** Base-metal thiolate complexes using ONS and SNS ligands: Synthesis and amine-borane dehydrogenation catalysis. **H. Keita**, U.K. Das, R. Baker

CHED **1138.** Immobilization of porphyrins in sol-gel matrices. **M. Schellman**, C.H. Lisse

CHED **1139.** Isomers and their interconversions for eight-coordinate, dodecahedral, rhenium(V) centers supported by four or five hydride ligands. **A. Scorzelli**, B. Macalush, G.A. Moehring

CHED **1140.** Influence of α-methyl substitution on nickel(II) complexes derived from 2-pyridinemethanamine. **S. Lozowski**, M.J. Prushan

CHED **1141.** Intramolecular hydrogen exchange at rhenium(V) pentahydride complexes stabilized by a primary amine ligand. **D.J. Streisel**, A. Petrou, G.A. Moehring

CHED **1142.** Synthesis and structural characterization of (dppp) $PtHSnPh_3$. **S. Hocharoen**, T.A. Mobley, K.E. Gilbert

CHED **1143.** Synthesis of Ru(II)(4,4′,4″-tritertbutyl-2,2′,6′,2″-terpyridine) catalysts for CO_2 reduction studies. **V. Caro**, T. Schneider, J. Nganga, A.M. Angeles Boza

CHED **1144.** Quaternary diamond-like sulfides: New candidate materials for infrared nonlinear optical devices. **M.M. Cribbs**, J. Glenn, J.A. Aitken

CHED **1145.** Synthesis of new rhodium catalysts for mechanistic investigation of dihydrogen evolution. **J. Hopkins**, Y. Peng, D. Lionetti, J.D. Blakemore

CHED **1146.** Progress towards tetradentate chiral metal complexes as Lewis acid catalysts. **B. Estepa Bernabeu**, C. Streu

CHED **1147.** Structural and spectroscopic studies of copper(II) complexes with ligands derived from 3,3'-Binicotinic acid. **R.J. Rabuska**, S.P. Watton, K. Jakobowski

CHED **1148.** Attempted synthesis and isolation of binuclear chromium quinone compounds for the purpose of oxidizing simple alcohols. **L.M. Whitt**, R.F. Johnston

CHED **1149.** Investigation of titanium complexes containing 2-iminoimidazoline ligands with sterically hindering side groups. **C. Mazzone,** J.K. Vohs

CHED **1150.** Sol-gel synthesis with applications to fireworks. **M.R. Glenn**, G. Gould, K.A. Woznack

CHED **1151.** Radiolysis of cosmic ice analogs of ammonia. **R. Tano-Menka**, **M. Thompson**, C. Arumainayagam

CHED **1152.** Fabrication and characterization of ceria-containing aerogels. **L. Posada**, M.K. Carroll, A.M. Anderson, B.A. Bruno

Section I

Moscone Center

Hall D

Undergraduate Research Posters

International Research Experience (IREU)

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1153.** Biomass derived furfuryl alcohol/water azeotrope as reaction medium for copper-catalyzed Ullmann-type condensation. **S. Fusi**, L. Vaccaro

CHED **1154.** Synthesis and modification of 4-hydroxyproline rich polypeptide oligomers. **M. Gaviria**, H. Arndt

CHED **1155.** Biogenic synthesis of silver nanoparticles using herb extracts. **L. Browder**, D. Yong Wei Ying, W.S. Chin

CHED **1156.** Investigating the biosynthesis of terrein in *Aspergillus terreus*. **M. Villanueva**, E. Skellam, R. Cox

CHED **1157.** Density functional theory: Determination of electrolyte redox potentials for rechargeable magnesium batteries. **A.T. Berry**, J. Mueller

CHED **1158.** Synthesis of super potent antibiotic cystobactamide 861-2. **A. Deyett**, A. Kirschning

CHED **1159.** Hydroxy-pyridine-carboxylate iridium complexes as extremely active, tunable and pH-responsive water oxidation catalysts. **R. Hutchinson**, G. Menendez Rodriguez, A. Macchioni

CHED **1160.** Attempts towards the preparation of substituted cyclohexane-1,3-diones as building blocks for dihydropyridine synthesis. **E. Janeira**, H. Arndt

CHED **1161.** Synthesis of cholesterol functionalized gold nanoparticles for the treatment of cardio vascular disease. **R. Kress**, D. Graham

CHED **1162.** Encapsulation of hydrophilic cargo within poly(lactic-*co*-glycolic acid) *micro- and nanoparticles*. **M.J. Austin**, S. Schubert, M. Leiske, A. Traeger, U.S. Schubert

CHED **1163.** Exploring the protein-protein interactions of PqsR in *Pseudomonas aeruginosa*. **K. Senn**, B. Woo, S. Chng

CHED **1164.** Investigating the optical properties of riboflavin interacting with metallic nanoparticles. **R. Warnock**, G. Massaro, L. Latterini

CHED **1165.** Mild two-step quaternization of amine-tethered metal-organic frameworks for anion-exchange applications. **M. Molenda**, Z. Hu, D. Zhao

CHED **1166.** P-docelyloxybenzyldimethylammine oxide (pDoAO) gel as pH sensitive artificial gland. **N.E. Caldero-Rodriguez**, P. Gentili

CHED **1167.** Novel composite material used as a lithium ion battery anode. **N. James**, C. Streb

CHED **1168.** Synthesis of novel conjugated small molecules based on 2,1,3-benzothiadiazole and 2,1,3-benzoxadiazole for organic photovoltaic applications. **M. Matar Abed**, J. Cameron, N. Findlay, P. Skabara

Section I

Moscone Center

Hall D

Undergraduate Research Posters

Medicinal Chemistry

Cosponsored by MEDI and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1169.** Synthesis and characterization of novel flavonoid derivatives as acetylcholinesterase inhibitors for the treatment of Alzheimer's disease. **J. DePhillips**, S. Martin, A. Denning, J. Minnick

CHED **1170.** T-0632 Amine analogs as potential agonists for the GLP-1 receptor. **C. Lepore**, G. Towers, D.R. Haines

CHED **1171.** Withdrawn.

CHED **1172.** Kinetics of doxorubicin degradation in various conditions. **C. Green**, E. Csuhai

CHED **1173.** Progress towards the synthesis of a novel bromo substituted aurone as a promising cyclooxygenase-2 inhibitor. **S. Forbes-Pentecost**, **M. Polk**, C. Mills, S. Stephenson

CHED **1174.** Disaggregation of lysozyme amyloid fibrils by combined drug delivery of curcumin and epigallocatechin gallate via multilayer Ca-alginate hydrogel micro-encapsulation. **A.J. Ferriol-Alonso**, C.M. Osorio-Cantillo

CHED **1175.** Structure-based drug design of novel therapeutics targeting metastatic breast cancer. **L. Hosek**, K. Tawara, M. King, D.L. Warner, C.L. Jorcyk

CHED **1176.** Thiamine as a carrier for drug delivery to cancer cells. **K. Hernandez**, J. Ayala-Rosa, S. Jarwan, S.H. Abdelwahed

CHED **1177.** Liquid-liquid extraction and analysis of the antioxidant, resveratrol, from red wine made at various fermentation temperatures. F.C. Mayville, **E.N. Sauschuck**, **A.M. Myers**

CHED **1178.** Investigation on the organometallic reagents involved in transmetalation of the Michael addition pertaining to artemisinin synthesis. **L.S. Gifford**, D. Fish

CHED **1179.** Synthesis and evaluation of ketone body esters for the treatment of neurological disorders. **E. Higgins**, S. Ulrich

CHED **1180.** Exploration of trans-2-(1,2,3-triazolyl)-cyclohexanols as potential inhibitors for fungal glycosidases. **M. Huey**, **B. Nguyen**, M.R. Ruyonga, N.M. Samoshina, V.V. Samoshin

CHED **1181.** Synthesis of multi-target ligands for the treatment of Alzheimer's disease. **K. Stupar**, D. Fish

CHED **1182.** Identification of new inhibitors for low molecular weight protein tyrosine phosphatase isoform A. **M. Olson**, H.V. Jakubowski, E.J. McIntee

CHED **1183.** Inhibition of CYP2A6 by alpha-substituted analogs of trans-cinnamic aldehyde. **G. Moyeen**, S. Black, K. Ebisuya, J.M. Chan, J. Harrelson

CHED **1184.** Effects of cannabinoids on TGFβ-complex protein, endoglin, in Ewing's sarcoma. **W. Willis**, J. Little, J. Rubin, M.D. Perry, L. Hensley

CHED **1185.** Progress towards the synthesis of aspernigrin A and structural analogs. **R.S. Arnold**, Z. Cross, D. Lemen, B. Marburger, L.M. Martin, D. McDermond, A.M. Reeve

CHED **1186.** Proteolytic activity of metal chelators as inhibitors of rattlesnake venom. **Y. Flores**, K. Combrink

CHED **1187.** Synthesis and toxicological analysis of 5' sulfamoylated adenosine scaffolds for *MtBPL* drug development. **M. Fuller**, M. Bockman, S. Dawadi, C.C. Aldrich

CHED **1188.** Assessing specificity of indazole derivatives as inhibitors to CYP2E1. **H. Hart**, G.P. Miller

CHED **1189.** Development of small peptidomimetic molecules targeting the CDYL2 chromodomain via massively parallel synthesis. **A. Estevez Davila**, S.V. Frye, K.D. Barnash, L.A. Ingerman

CHED **1190.** Poly(ethylene glycol) functionalized-4',4"-diflurobenztropine analogues. **E. Houchen**, N.M. Paul

CHED **1191.** Progress toward the synthesis of a photosensitive ALK5 inhibitor. **J. Newson**, A. Rola, C. Streu

CHED **1192.** Infection of T follicular helper cells during acute SIV infection of infant macaques by the oral route. **M. Warren**, B. Phillips, K. DeParis

CHED **1193.** Ionic liquids as antimicrobial materials. **C. Migliori**, **D. Stapleton**, J. Melessa, K. Merrett, L. Simmons, Z. Pearson, G. Ifijeh, A. Everett, A. Young, D. Warner, D. Fox, A.T. Koppisch, R.E. Del Sesto

CHED **1194.** Synthesis of novel ALK5 inhibitors. **T. Hall**, L. Kelsey, C. Streu

CHED **1195.** Design and synthesis of a non-covalent macrocyclic proteasome inhibitor. **M. Palmer**, R. Dorn, M. Rocha, G. Merrill-Steskal, M.G. Gotz

CHED **1196.** Acid-labile oleoyl-PEG orthoester micelles for controlled drug delivery. **F.M. Ippoliti**, L.E. Prevette

CHED **1197.** Investigating leaving group effects towards a covalently binding Toll-like receptor agonist. **A. Bhattacharya**, A.C. Chon, A.P. Esser-Kahn

CHED **1198.** De novo design of novel NOP receptor agonists for the treatment of post-traumatic stress disorder. **M.R. Koebel**, A. Cooper, S. Sirimulla

CHED **1199.** Identification of potentially novel antimicrobial molecules produced by isolated *Streptomycetes*. **M. Almaraz**, G. Palmer

CHED **1200.** Extraction, quantification, and antioxidant analysis of annonacin from fruit of the North American Pawpaw (*Asimina triloba*). F.C. Mayville, **E.C. Charamut**, C.R. Kovaleski

CHED **1201.** Withdrawn.

CHED **1202.** Using light to kill cancer-development of a novel photodynamic therapy agent. **A. Hamiton**, J.E. Bradshaw

CHED **1203.** Possible breast cancer photodynamic therapy agents: H_2TPP-A4OH and H_2TPP-A6OH. **M. Richards**, J.E. Bradshaw

CHED **1204.** Targeted Inhibition of COX-2. **C. Armstrong**, C. Streu

CHED **1205.** Explaining chemical space with light: Light-activated molecules to probe biosystems. **M. Zafferani**, **C. Streu**

CHED **1206.** Metal chelate inhibitors of rattle snake venom. **J.G. Escobar**, K. Combrink

CHED **1207.** Synthesis of nonsteteroidal analogs of CAmSA as anti-*Clostridium difficile* agents. **A. Taylor**, I. Donkor

CHED **1208.** Design and synthesis of novel liver X receptor ligands. K.A. Payne, **K.M. Lamark**, D.A. Spadoni, D. Adams, R. Komati, K. Riley

CHED **1209.** Rifamycin derivatives to treat *Mycobacterium abscessus*. **K.N. Elizondo**, K. Combrink, A. Ramirez-Ramos, S. Spring, F. Maurer

CHED **1210.** Synthesis of oxazolidinones containing tricyclic fused rings. **M.C. Audi**, **T. Lesmeister**, **A.N. Roux**, J.T. Ippoliti

CHED **1211.** Synthesis of potential AAC(6')-Ib inhibitors to combat bacterial resistance to aminoglycoside antibiotics. **M. Simes**, L. Miers, K.J. Labby

CHED **1212.** Effects of FDA-approved compounds on biofilm formation and antibiotic sensitivity in *Staphylococcus haemolyticus*. **L. Nguyen**, M.S. Blackledge

CHED **1213.** Development of a medicinal chemistry lab to demonstrate the effects of molecular weight and polarity on lipophilicity. **A. Schrader**, B. Buckner, M. Manpadi

CHED **1214.** Synthesis of several polyamine analogs as possible growth inhibitors for breast cancer cells. F.C. Mayville, **E. Phillips**, **E. Brown**, **A.L. Bielski**

CHED **1215.** Fragment library docking with HADDOCK: Identifying protein binding hotspots and improving site sampling. **E. Elder**, A. Bonvin, J. Grinstead

CHED **1216.** Effect of cannabinoid treatment on CD99 expression in Ewing's sarcoma. **D. Dwelle**, L. Hensley

CHED **1217.** Synthesis and structural analysis of novel quercetin antioxidant and antitumor agent: Antitumor activity on mouse T2A and T3PA cancer cells. **E. Tharnish**, C. Parry, A. Thomas, M. Grossmann, C. Kriley, M.M. Majireck, E. Reinheimer

CHED **1218.** Dual COX-2/sEH inhibitor treats kidney damage in type 2 diabetic rats. **K. Craig**, A. Khan, J. Imig

CHED **1219.** Investigation of FDA-approved small molecules as modulators of virulence in Methicillin-Resistant *Staphylococcus aureus* (MRSA). **K. Gillard**, T. Wilson, P. Vigueira, A. Sarkar, M.S. Blackledge

CHED **1220.** DNA intercalation and Topoisomerase I inhibition studies of aryl sulfoxides. **A. Jefferys**, A. Hurley Predecki

CHED **1221.** Computational and SRB analysis of novel naphthoquinone analogues. **B. Tuhlei**, M. Manpadi, Z. Medcalf

CHED **1222.** Synthesis and analysis of tautomerically ambiguous cytosine-based analogs to induce viral mutagenesis. **C.M. Clem**, W.R. Fernandez, S.M. Hardage, S.E. Kuhn, V.K. Dunlap

CHED **1223.** Cellular response to spider silk scaffolds. **D. Montag**, K. Hafner, M. Kennedy, D. Dean

CHED **1224.** Computational simulations of chiral drug metabolism by mutated CYP2C9. **A. Holcomb**, G.P. Miller, M.D. Perry

CHED **1225.** Mechanistic study of genetic response induced by novel naphthoquinone analogues. **D.B. Sitapara**, A. Delawder, J. Sparks, M. Manpadi

CHED **1226.** Small molecule modulation of virulence behaviors in *Staphylococcus epidermidis*. **R. Ulrich**, M. Behrens, M.S. Blackledge

CHED **1227.** Expression of β-catenin from diabetic and cancerous cells in the presence of glucose. **R. Stahl**, K.S. George Parsons

CHED **1228.** Novel excipients that reduce the viscosity of concentrated monoclonal antibody formula novel excipients that reduce the viscosity of concentrated monoclonal antibody formulations. **H.F. Gezahagne**, A.M. Larson, A.K. Weight, K. Love, C. Wescott, A. Bonificio

CHED **1229.** Pillaring classic honeycomb SBLs as a method to 3-periodic MOFs. **E.A. Alonso**, J.F. Eubank

CHED **1230.** Isolation of curcuminoids from turmeric *Curcuma longa*. **S.A. Saey**, N.Y. Ayala, B.E. Sturgeon

CHED **1231.** Evaluation of antimicrobial properties of *Combretum laxum extracts*. **J.G. Escobar**, A.K. Addo-Mensah

CHED **1232.** Synthesis and study of triple-headed, double-tailed amphiphiles as potent antiseptics. **S.D. Kendrick**, R. Elizabeth, K. Seifert, K.L. Caran

CHED **1233.** Synthesis of novel casein kinase 1 inhibitors for treatment of Alzheimer's disease. **C. Gettridge**, J. Sridhar

CHED **1234.** *In vitro* studies on non-toxic polysaccharide based drug/gene delivery systems: Safety/toxicity studies. R. Srinivasan, **L. Hernandez**, **J. Murphy**, **J. Orona**

CHED **1235.** Changes in mechanical and chemical properties of rat femur and tibia bones exposed to simulated microgravity and cosmic radiation. **H.N. Heacox**, R. Mehta, B. Hill, P. Chowdhury, M. Dobretsov, L.M. Benzmiller, J. Barajas, S. Freyaldenhoven

CHED **1236.** Energetics of molecular recognition of substituted-warfarins by serum albumin as a model for blood ADME drug properties. **E. Munyaneza**, E.J. Valente, K.M. Bishop, **R. Bishop**

CHED **1237.** Molecular diversity of kavalactones from kava-kava root extractions. **R. Bishop**, **M.A. Bowser**, **K.N. Brunk**, **L.C. Bishop**, E. Munyaneza, K.M. Bishop

CHED **1238.** Progress on the synthesis of a methotraxate-phenylalanine derivative for the treatment of glioblastoma in antibody-directed enzyme prodrug therapy. M.J. Rouffet, **S. Frantz**, **P. Katherine**, M. Dorrell

CHED **1239.** Chemical analysis and antimicrobial activity of Maine *Ulva lactuca* after prolonged storage. **J. Woolf**, A.M. Deveau, K.M. Burkholder, Z. Miller-Hope, C. Russell, E. Lloyd

CHED **1240.** Anti-bacterial synergy of medicinal herbs. **B. Niemi**, **A.B. Waghe**

CHED **1241.** Synthesis and analysis of MTN inhibitors: A potential new class of antibiotics to treat drug resistant infections. **R.B. Mukuna**, H. Dossett, N. Hunter, P. Erstad, D. Xu, J.H. Thurston, K. Cornell

CHED **1242.** Accumulation of phytochemical compounds in *Calendula officinalis* grown under differential light and nitrogen conditions. **P. Tuladhar**, S. Shrestha

CHED **1243.** Isolation and modification of mithramycin SA. **L. Hartline**, P. Daniels, S. Brooks, A. Foster, D. Scott

CHED **1244.** *Heracleum maximum and Psoralea corylifolia:* Toxicity/phototoxicity evaluation. **B. Pinsky**, **G. Jones**, **C. King**, J. Hoffmann, M. Morrow, P. Dhar

CHED **1245.** Synthesis of 2-(2-trifluoromethylsulfonamido)phenylbenzimidazole derivatives as potential IspF inhibitors. M.J. Rouffet, **C. Dunham**

CHED **1246.** Enhancing antibacterial properties using herbal extracts. **J. Knapp**, **A.B. Waghe**

CHED **1247.** Antibiotic and hyaluronidase-inhibiting fractions from the *Rhododendron* flower. **R. Wetzel**, A. Hoffman

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Nanochemistry

Cosponsored by SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1248.** EPR Characterization of incorporated membrane proteins into StMA-lipid nanoparticles. **A. Bali**, A.F. Craig, I. Sahu, D. Konkolewicz, G. Lorigan

‡ *Cooperative Cosponsorship*

CHED **1249.** Employ of nanotechnology as a resource of improvement for the agricultural sector: Enhancement on the early growth of *Abelmoschus esculentus* treated seeds using green synthesized gold nanoparticles. **J. G. Noel-Torres**, C.N. Burgos-Feliciano, C. Pellicier-Rodriguez, C.M. Osorio-Cantillo

CHED **1250.** Synthesis of functionalized superparamagnetic cobalt ferrite nanoparticles and optimization for specific phosphoprotein enrichment. **K. Dani**, B. Chen, S. Jin

CHED **1251.** Infrared and surface-enhanced infrared absorption study of dopamine adsorption on Cu nanostructures. **M. Lindsey**, D. Perry

CHED **1252.** Synthesis and characterization of core/shell, copper indium sulfide/silver gallium sulfide nanocrystals. **E. Searles**, S. Hughes

CHED **1253.** Developing methods to examine the toxicity of $CuInS_2$/ZnS nanocrystals using *Danio Rerio (zebrafish) embryos*. **C. Peterson**, S. Hughes

CHED **1254.** Control of the surface density of thioctic acid on gold nanoparticles and its effect on stability and catalytic activity. **A. Crawford**, J. Park

CHED **1255.** Use of scanning tunneling spectroscopy to characterize doped ZnO nanorods for solar cell applications. **A. Carr**, E. Adcock Smith, J.A. Phillips, K. Roberts, E.V. Iski

CHED **1256.** Application of thermally stable silver halide monolayers to polycrystalline gold. **H.R. Morgan**, L.E. Jackson, J.A. Phillips, E.V. Iski

CHED **1257.** Effect of gold nanoparticles and sudafed on Daphnia Magna. **J. Chabrier Rodriguez**, R.M. Perez-Ortiz, N. Cardona, P. Ostolaza, J.I. Ramirez Domenech, E. Ferrer Torres

CHED **1258.** Synthesis and characterization of mesoporous zirconia. **J. Roach**, D.S. Heroux

CHED **1259.** Neurodevelopmental toxicity of low concentration silver nanoparticles in embryonic zebrafish (*Danio rerio)*. **T. Hemphill**, V. Nicolae, A. Latta, S. Robertson, R. Manteca, C.C. Pena, J.J. Pak, M.A. Thomas, J.D. Harris

CHED **1260.** Investigation of mixed monolayer systems on Au(111). **D. Fitzgerald**, E. Krisanda, **C. Szypko**, G. Avila-Bront

CHED **1261.** Novel characterization of silver & gold nanoparticles utilizing a laser system. **R. Maharaj**, M.O. Montes, K.A. Beran

CHED **1262.** Effect of ZnO nanoparticle morphology on photodegredation of Janus Green B Azo Dye. **H.V. Anderson**, C.C. Pena, J.D. Harris, J. Cowan, J.J. Pak, J. Croteau, D. Butt

CHED **1263.** Enhancing drug delivery using antibiotic-incorporated silver nanofibers. K. LaiHing, **J. Lewis**, **A. White**

CHED **1264.** Synthesis of magnetic nanoparticles for biomolecule attachment and future biosensors. **K. Burch**, G. LeBlanc, D. Wirth

CHED **1265.** Characterization and photothermal effects of gold nanoparticles with gallic acid ligands. **E. Evans**, E. Hysi, B. Mellis

CHED **1266.** Effects of silver nanoparticles and orphenadrine on Daphnia Magna. **G.M. Santiago Rivera**, Y. Santos-Vazquez, R.M. Perez-Ortiz, E. Ferrer Torres, J.I. Ramirez Domenech

CHED **1267.** Synthesis and characterization of Au:Ag core-shell nanoparticles with 4-aminothiophenol Surface Enhance Raman Spectroscopy (SERS) tag. **M. Gladding**, B.D. Gilbert

CHED **1268.** Stability of insulin bound on nanodiamonds. **A.T. Arshi**, B. Negru, M. Su, H. Shi, I. Jones

CHED **1269.** Azide functionalization of nanoporous gold. **N.J. Chevalier**, **D.T. Favre**, E.C. Landis

CHED **1270.** Synthesis and characterization of quantum dot@hexaniobate nanopeapods. **K. Moore**, T.T. Brown, J.B. Wiley

CHED **1271.** Identification of novel folate-binding proteins. **K. Holton**, L.M. Watkins

CHED **1272.** Silver halide monolayers: An EC-STM study of stability on a Au(111) surface. **L.E. Jackson**, J.A. Phillips, H.R. Morgan, G.H. Jones, E.V. Iski

CHED **1273.** Characterization of DAPI and PACA as novel, hidden, tag molecules for SERS spectroscopy of silver-coated, gold nanoparticles. **V. Wood**, B.D. Gilbert

CHED **1274.** Synthesis and characterization of redox-responsive porphyrin-loaded polysilsesquioxane nanoparticles for photodynamic therapy. **C.N. Mena**

CHED **1275.** Electrochemical control of phase change properties in nanoparticles of silver selenide. **J. Yungbluth**, G. LeBlanc

CHED **1276.** Soft microspheres with discrete fluorescent nanospheres for measuring forces during phagocytosis. **D. Hay**, B. Evans

CHED **1277.** Growth of *Shewanella oneidensis* in the presence of toxic metals: A basis for sustainable semiconducting nanoparticle biosynthesis. **A.M. Bell**, S. Lampa-Pastirk

CHED **1278.** Synergistic enhancement of antibiotic activity with silver nanoparticles. **E. Stuffle**, G. Vildor, C. Stewart, K. LaiHing

CHED **1279.** Nanodiscs stabilize *Anabaena* sensory rhodopsin trimers for regulatory binding studies. **A. Aguiar**, **J.M. Massey, J. Andersen**, E. Sandoval, J.A. Cappuccio

CHED **1280.** Study of metalloporphyrins on gold surfaces via scanning tunneling spectroscopy. **L. Joseph**, D. Del Sesto

CHED **1281.** Investigating the hard corona of novel nano-vehicles in model biological fluids. **A.W. Cheema**, N.T. Flynn, A.C. Webb

CHED **1282.** Binding and thermodynamic studies of myoglobin with polyethylene glycol coated iron oxide nanoparticles. **A. Vanyo**, A. Fazal

CHED **1283.** Effect of polyethylene glycol-coated magnetic nanoparticles on the catalytic activity of myoglobin. **A.A. Charbonneau**, A. Fazal

CHED **1284.** Using plasmon molecular resonance to increase LSPR sensitivity. **A. Gray**, P. Hall-Osberg

CHED **1285.** Chemical modifications to tailor electronic structure of 2-dimensional nano-materials. **S.S. Esdaille**, T. Schiros

CHED **1286.** Comparing the synergistic enhancement of antibiotic activity between biologically and chemically synthesized silver nanoparticles. **G. Vildor**, K. LaiHing

CHED **1287.** Infusion of silver-gold bimetallic nanoparticles in organic nanofibers for antimicrobial use. **C. Stewart**, E. Stuffle, K. LaiHing

CHED **1288.** Gold nanoparticle depuration in wood frog (*L. sylvaticus)* tadpoles after post-exposure habitation in fresh water. **K.T. Lerner**, P.P. Fong, L.B. Thompson

CHED **1289.** Incorporation of silver-based antibiotic in organic nanofibers for drug enhancement. K. LaiHing, **A. Saunders**, **S. Parkins**

CHED **1290.** SERS detection of graphene oxide in acid-catalyzed sol-gels. **B. Wyatt**, E.J. Atkinson

CHED **1291.** Monolayer deposition of colloidal quantum dots by spray-coating. A.S. Abrams, **R.E. Mow**, **G.P. Murray**, S.H. Tan, H. Van Ryswyk

CHED **1292.** Scattering mediated absorption in photonic crystals. **N. Eldabagh**, J.J. Foley, K.R. Fernando

CHED **1293.** Synthesis of gold and silver nanotriangles using plant extracts. **D. Perillo**, M. Schiza

CHED **1294.** Quantifying the thermodynamics of the surface modification of oleate-capped CdSe quantum dots with dodecylphosphonic acid via isothermal titration calorimetry. **Z.B. Di Giusto**, J.D. Keene

CHED **1295.** Hierarchical SnS nanostructures for efficient energy devices. **A.M. DeGrauw**, L.L. Whittaker

CHED **1296.** Effect of silver nanoparticles on migratory properties of cultured fibroblasts. **O. Creech**, L. Seballos, B. Sharma

CHED **1297.** Quantum dot growth using cysteine polymers in a one pot method. **S. Yang**, R. Nevarez, M. Garica, I. Gasparyan, Y. Nowry, P. Lee

CHED **1298.** Effect of capping agents on the antibacterial properties of silver nanoparticles. **H.P. Nguyen**, A.L. Smalley

CHED **1299.** Hybrid dual-layer zinc oxide dye-sensitized solar cells. **C. Tan**, K.W. Huang, H. Van Ryswyk

CHED **1300.** Covalent immobilization of graphene on patterned SAMs for investigation of frictional properties. **M.L. Grandon**, M.B. Elinski, M. Negrito, Z. Liu, J.D. Batteas

CHED **1301.** Hydrothermal synthesis and characterization of two dimensional tin sulfide nanosheets. **E. Juarez Diaz**, Y. Zayas Ortiz, N. Trejo, J.D. Dwyer, E.S. Aydil

CHED **1302.** Nanotechnology and art in chemical education. **J. Garcia**, **J. Liu**, **E. Chan**, **F. Schwebel**, **F. Mongue**, **J. Blatti**, A. Quinonez, T. Kwan

CHED **1303.** Partially poisoned palladium nanoparticles for selective chemical conversion: Hydrogenation of C=C bonds. **H. Nguyen**, Y. Shon

CHED **1304.** Temperature effects $_{60}$on C_{60} fullerene in alkane, alkene, fatty acid, and vegetable oil solutions. L.D. Bienski, C.L. Aronson, **R. Ferrer**, **L.A. Pajarillo**, **B.S. Blackwell**, **J. Ballard**, **M. Kennedy**, **V. Te**

CHED **1305.** Gingivitis prevention: Integration of iron (II, III) oxide nanoparticles into commercial mouthwash. **J. Nguyen**, M. Osinski

CHED **1306.** Effect of fluoxetine-conjugated gold nanoparticles on aquatic organisms. **R.J. Gawel**, P.P. Fong, L.B. Thompson

CHED **1307.** Quantification of polyelectrolyte adsorption to gold nanoparticle surfaces. **C.M. Harris**, **F.E. McFeaters**, K. Andresen, L.B. Thompson

CHED **1308.** Raman characterization of binary hydrates. **K. Keefe**, N. Ismail, C.A. Koh

CHED **1309.** Towards improving drug delivery technology with dual-payload gold nanoparticles. **C. Akers**, D. Scott

CHED **1310.** Seeded synthesis of nanomites by combining top-down and bottom-up strategies. **W.E. Scholl**, C.A. Lancaster, M.A. Ticknor, J.S. Shumaker-Parry

CHED **1311.** Creation of PEG-capped aluminum nanoparticles for tissue engineering and energetics applications. **I. Stochl**, S. Sell, S.W. Buckner, P.A. Jelliss

CHED **1312.** Study of the Impact of surface charge of silica nanoparticles on enhanced oil recovery (EOR). **L.M. Aponte- Reyes**, L.M. Aponte-Cruz, P. Loman-Cortes, J.L. Vivero-Escoto, M.P. Alvarez

CHED **1313.** Characterizing the nanomechanical properties of β-amyloid aggregation on various lipid surfaces by atomic force microscopy. **B.S. Flaherty**, E.A. Yates

CHED **1314.** Gold nanoshapes synthesis for surface enhanced Raman applications. **M. Snyder**, M. Schiza

CHED **1315.** Doping of 2D nanomaterials: Investigation of chemical environment and electronic structure effect. **N. Cassel**, W. Archibald, S. Sambasivan

CHED **1316.** Interactions of myoglobin with nanodiamond particles. **C. Sylvia**, B. Negru, M. Su, H. Shi, I. Jones

CHED **1317.** Art of adsorption: Protein attachment onto charged nanodiamonds. **S.M. Trikha**, B. Negru, M. Su, H. Shi, I. Jones

CHED **1318.** Novel solution for powering our planet: Comparative study of a novel titania sol and a titania powder for the improved efficiency of dye-sensitized solar cells. **L. Joseph**, L. Klein

CHED **1319.** Ultraviolet-Visible characterization of Buckminsterfullerene C_{60} dissolved in organic monomersπ. C.L. Aronson, L.D. Bienski, **L.A. Pajarillo**, **B.S. Blackwell**, **Z. Jones**, **R. Muzquiz**, **C. Anding**, **M. Bryant**, **R. Ferrer**

CHED **1320.** Synthesis of fluorescent, gallic acid capped gold nanoparticles. **K. Vazquez**, J. Hollingsworth, W. Crawford, B. Mellis

CHED **1321.** Effect of Ligand Identity on Quantum Dot Sensitized Solar Cell Performance. **N. Hendrix**, J. Snyder, K. Schnitzenbaumer

CHED **1322.** Microwave assisted growth of cobalt doped ZnO nanorods. **S. Huang**, E. Adcock Smith, K. Roberts

CHED **1323.** Evaluation of the effect of Ag, Au and ZnO nanoparticles on the kinetic of degradation of allura red AC and brilliant blue FCF dyes in wastewater. **A. Rosado-Torres**, J. Pacheco-Torres, J. Tirado-Robles, M. Santiago-Mercado, C.M. Osorio-Cantillo

CHED **1324.** Metallic nanoparticle production by CVS probiotic. **H. Peng**, M.O. Montes

CHED **1325.** Glycerol mediated synthesis and applications of silver citrate nanoparticles. **V.M. Wartenweiler**, S. Laing, H. May

CHED **1326.** Infrared and surface-enhanced infrared absorption study of dopamine adsorption on silver nanostructures. **G. Cartwright**, D. Perry

CHED **1327.** Synthesis of gold, silica and silica@gold core shell nanoparticles for functionalization with anti-cancer drugs. **F.D. Rodriguez**, **N.N. Sosa Cintron**, E. Ferrer Torres, M.P. Alvarez, C. Osorio Cantillo

CHED **1328.** Effect of the interaction of ZnO nanoparticles and the gentamicin in growing populations of *Staphylococcus aureus*. E. Ferrer Torres, **S. Figueroa Gonzalez**, C. Osorio Cantillo, J.I. Ramirez Domenech

CHED **1329.** Stabilization of 4',6-Diamidino-2-Phenylindole (DAPI) in base-catalyzed sol-gels containing silver nanoparticles vs. solution using Surface Enhanced Raman Spectroscopy (SERS). **D. Mason**, E.J. Atkinson

CHED **1330.** Surface-Enhanced infrared absorption studies of copper nanostructures formed by oblique-angle deposition. **B. Branch**, D. Perry

CHED **1331.** Development of nanomaterials research project at a community college. **J. Orozco**, **D. Mikhail**, **M. Ramos**, **S. Sanders**, B. Bekker, S. Fan

CHED **1332.** Withdrawn.

CHED **1333.** Synthesis, characterization and antimicrobial activity of drug-loaded calcium alginate nanocapsules: Perspectives on their potential biomedical use. **A. Anaya,** T. Palacios-Hernández, M. Méndez-Rojas, A. Aburto Platas

CHED **1334.** Study of protein-nanodiamond attached on silica surface with attenuated total reflection spectroscopy. **M. Hallberg**, B. Negru, M. Su, H. Shi, I. Jones

CHED **1335.** Electrooptical dynamics of 4-cyano-4'-pentylbiphenyl mounted on ZnSe functionalized with alkanethiol self-assembled monolayers. **E.C. Rossomme**, A.R. Noble

CHED **1336.** Antibacterial properties of metallic nanoparticle-doped MOFs in water. **J. Walker**, K. Couser, N. Le, K.T. Jackson

CHED **1337.** Colloidal synthesis: A route towards nanometric cathode material for mutivalent batteries. **J. Bolotnikov**, G. Nolis, J. Cabana

CHED **1338.** Toxicological study of green synthesized silver and gold nanoparticles on germination and early lengths of *Sesamum indicum* seeds. J. Pacheco-Torres, M. Santiago-Mercado, **C. Torres-Martinez**, C.M. Osorio-Cantillo

Section I

Moscone Center

Hall D

Undergraduate Research Posters

Organic Chemistry

Cosponsored by SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1339.** Directed solid phase peptide synthesis of α-conotoxin MII. **J. Fothergill**, O.M. McDougal

CHED **1340.** Synthesis of quinoxalines and the analysis of their bond lengths via x-ray diffraction. **J. DiSapio**, **R. Van Wart**, G.A. Crundwell, N.M. Glagovich

CHED **1341.** Design and synthesis of cyclic dipeptides for biomimetic epoxidation. **C.R. Drisko**, K.S. Huang

CHED **1342.** Synthesis and metalation of *N*-methylbenzocarbaporphyrins. **A.N. Latham**, T.D. Lash

CHED **1343.** Ozonolysis of cycloalkenes in the presence of unsaturated nucleophiles: Synthesis of tri-functional aldehyde-ester-alkene compounds. **D.P. Soulsby**, J. Ung

CHED **1344.** Novel synthesis methods for naturally occuring THF derivatives. **G. Pombar**, Y. Yuan

CHED **1345.** Exploring sequence effects in cucurbit[n]uril-peptide interactions. **Z. Hirani**, E.F. Babcock, A.R. Urbach

CHED **1346.** Effects of neighboring sequence context on cucurbit[n]uril-peptide interactions. **E.F. Babcock**, Z. Hirani, A.R. Urbach

CHED **1347.** One-pot dialkylation of cycloalkanones and their ring-closing metathesis to make bridged bicyclic compounds. **D. Sacenti**, **A. Yoon**, J.B. White

CHED **1348.** Stereoselectivity of stilbene synthesis by palladium-catalyzed Heck reaction. **K.J. Clark**, N.S. Werner

CHED **1349.** Rapid synthesis of *N*-(4-isopropylbenzyl)-*N*-methylformamide. **S. Sundhagen**, L.I. Bobyleva, M.M. Bobylev

CHED **1350.** Examining syntheses and photochemical reactivity of 5,6-diethynylquinoxalines. **A.J. Cortes**, B.F. Gherman, J.D. Spence

CHED **1351.** C^1-C^7 Diradical cyclization of an anthracen-9-yl substituted enyne-enone. **M.R. Hutchinson**, B.F. Gherman, J.D. Spence

CHED **1352.** Investigating cyclization channels of substituted enyne-enone derivatives. **F. Sakdamart**, B.F. Gherman, J.D. Spence

CHED **1353.** Alterating scents: Modifying the ionones and studying the effect on fragrance. **S. Crosio**, J.D. Pike

CHED **1354.** Developing a colorimetric competitive displacement assay to screen for catalytic peptides. **A. Gest**, L. Witus

CHED **1355.** Synthesis of silylated tetrahydropyrans from organosilanes. **J. Hampton**, A. Diez-Varga, C. Díez-Poza, V. Díez-Lebrato, G. González-Gil, A. Barbero

CHED **1356.** Synthesis and characterization of mixed short and medium chain fatty acid triacylglycerols. **G. Cabrera**, R.P. D'Amelia, W.F. Nirode, L. Huang

CHED **1357.** DNA-templated synthesis of macrocycles. S. Griffin, **K.S. Huang**

CHED **1358.** One-pot synthesis of tetramisole-derived organocatalysts from amino alcohols. **R. Morris**, M. Paeth, P. Willoughby

CHED **1359.** Progress toward the synthesis of deoxypodophyllotoxin. **B. Rencher**, D.I. Saavedra, M. Andrus

CHED **1360.** Assessment of the handedness of *ortho-phenylene* folding. **R. Pandian**, G. Vemuri, C. Hartley

CHED **1361.** NMR analysis of pyrrolizidine alkaloid monoesters from the plant family Boraginaceae. **C.J. Burghard**, **P. Cantrell**, **L. Johnson**, R.B. Kelley

CHED **1362.** Progress towards the synthesis of F4-4. **P.J. Hurst**, D.I. Saavedra, M. Andrus

CHED **1363.** Gold-catalyzed cycloetherification of epoxides. **T. Silva**, J.R. Vyvyan

CHED **1364.** Mechanistic investigation of the formation of *N*-sulfonyl aldimines from aldehydes and iminoiodinanes. **K.A. Scott**, M.D. Hopkins, B. DeMier, A.A. Lamar

CHED **1365.** Investigation of the effect of iminoiodinane reagent on the synthesis of *N*-sulfonyl aldimines from aldehydes. **B. DeMier**, M.D. Hopkins, K.A. Scott, A.A. Lamar

CHED **1366.** Mild chlorination of arenes using organic dyes as visible-light photoredox catalysts. **A.T. Bensalah**, A.A. Lamar

CHED **1367.** Rapid synthesis of *N-methyl-N*-(4-trifluoromethylbenzyl)formamide. **S. Park**, L.I. Bobyleva, M.M. Bobylev

CHED **1368.** Rapid synthesis of *N-vanillylbutyramide*. **J. Choi**, L.I. Bobyleva, M.M. Bobylev

CHED **1369.** Synthesis of calcitroic acid to determine its potential for prevention of colon cancer. **V. Senych**, O.B. Yu, L. Arnold

CHED **1370.** Extending the substrate scope of the Chan-Lam cross-coupling reaction using photoredox catalysis. **J. Marshall**, A.J. Wommack, A. Schiro

CHED **1371.** Synthesis and nucleic acid binding applications of diversely functionalized macrocyclic heteroarylopeptoids. A.A. Fuller, **C. Bosmajian**, A. Mohan

CHED **1372.** Synthesis of indolyl/indazolyl (N1 substituted) quinolones (C6 substituted) for study as possible anticancer/antibiotic/antimicrobial agents. **L. Ito**, **K. Reicher**, **P. Schulzetenberg**, T.M. Trygstad

CHED **1373.** Induced-fit binding of cucurbit[7]uril to insulin B1-11 in aqueous solution. **A.R. Karla**, A.R. Urbach

CHED **1374.** Applying a new amination method for the efficient synthesis of calothrixin B. **M. Dekarske**, L.M. Mori Quiroz, M.D. Clift

CHED **1375.** Synthetic receptors and cyclic peptides. **E. Boms**, A.T. Bockus, A.R. Urbach

CHED **1376.** PIB-bound pybox ligands. **M. Gulley**, T. Malinski, D. Bergbreiter

CHED **1377.** Convergent synthesis of *trans-alkene peptide isosteres*. **S.E. Huth**, B.R. Sculimbrene

CHED **1378.** Enantioselective catalytic phosphorylation. **P.J. Endres**, B.R. Sculimbrene

CHED **1379.** Novel route to acridines. **K. Berger**, J. Jaye, G. McCormick, E.H. Fort

CHED **1380.** Kinetic scheme of the decarboxylative cross-ketonization of carboxylic acids with zirconia catalyst. **O.A. Fraser**, A. Cohen, A. Ignatchenko

CHED **1381.** Analysis of the structure activity relationship between novel malonamides and their fluorescence characteristics. **B.I. Gomez**, J. Jennings, A.K. Franz

CHED **1382.** Destruction of organophosphorus nerve agents using metal-organic frameworks. **C. Whitaker**, A. Brady, L. Webb

CHED **1383.** Synthesis and photophysical studies of solvatochromic compounds containing fluorene-quinoxaline donor-acceptor chromophores. **S.R. Johnson**, **L.M. Wickham**, J.M. Nadeau

CHED **1384.** Synthesis of thioether-substituted dibenzo[*fg,op*]naphthacene liquid crystals. **C. Henry**, P. Repasky, C. Hartley

CHED **1385.** Synthesis of a perylenebisimide ligand for improving the light absorption properties of luminescent solar concentrators. **H. Towns**, R.C. Chambers

CHED **1386.** Controlling the handedness of *ortho*-phenylene helices through substitution at the termini. **E.B. Stopler**, G. Vemuri, C. Hartley

CHED **1387.** Synthesis and photocharacterization of a photodynamic oxytocin antagonist. **R. Ryan**, C. Streu, M. Kazmierczak

CHED **1388.** Solid-state studies of benzonitrile oxides and their dimers: Crystal structure of a 1,2,4-oxadiazole. **M. Neuzil**, W.H. Ojala

CHED **1389.** Solid-state structures and reactivity of halogenated benzonitrile oxides: Crystal structure of *bis*(3-chlorophenyl)furoxan. **M. Stodolka**, W.H. Ojala

CHED **1390.** Solid-state chemistry of dimers of a sterically hindered benzonitrile oxide. **K. Idzorek**, W.H. Ojala

CHED **1391.** Synthesis of a PFTase substrate containing a terminal olefin capable of tetrazine ligation. **S. Auger**, J. Wollack

CHED **1392.** Evidence for formyl and α-hydrogen bonding in asymmetric organic reactions from single crystal X-ray diffraction and density functional theory. **J. Cosme-Silva**, J.D. Evanseck, J. Rohde, B. Vernier, M. Novak, M. Kanzelberger

CHED **1393.** Bioorthogonal synthesis of novel fluorophores. **S.S. Rubeck**, X. Shang, J. Guo

CHED **1394.** Synthetic methedologies for pyrazolones analogues as potential drug candidates for pulmonary fibrosis. **T. Bader**, C.P. Jasperse, H. Abdulsalam

CHED **1395.** Development of new analgesic drugs. **M. Langereis**, M. Hossain

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

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CHED **1396.** *N*-Heterocyclic carbene-catalyzed conversion of α-amino alcohols to their corresponding epoxides. **S.T. Goralski**, B.M. Saliba, K.R. Overly

CHED **1397.** Natural products to combat leishmaniasis: Synthesis of espinatol-based anti-parasitics. **A.T. Hargis**, G.R. Naumiec

CHED **1398.** Use of peptoids for the detection of aromatic water contaminants. A.A. Fuller, **K. Tenorio**, **J. Huber**

CHED **1399.** Synthesis of macrocyclic aromatic oligoamides. A.A. Fuller, **D. Tiano**, **J. Tobias**

CHED **1400.** Synthesis of 3-alkoxybenziporphyrins. **R.A. Tomlovich**, T.D. Lash

CHED **1401.** Synthesis and characterization of 5-(3'-thienyl)pentanoic acid capped lead sulfide nanoparticles for polymeric photovoltaic cells. **M.J. Strauss**, R.W. Kopitzke, J. Zemke

CHED **1402.** Synthesis of heterodisubstituted pyridines via cyclization of methyl ketones, DMSO, and ammonium salts. **H. Cole**, H. Clause, B. Bowers, S.K. Goforth

CHED **1403.** Synthesis of *O*-acylated amino acid surfactants with hydrophobic ω-alkenyl chains. **C. Young**, **A.P. Szczepanski**, D. Brownholland

CHED **1404.** Microwave-assisted gold(I)-catalyzed Friedel-Crafts-like arylation of benzylic alcohols to afford 1,1-diarylmethanes. R.G. Iafe, **J.V. Oakley**, T. Stanley

CHED **1405.** Synthesis of silylethynyl substituted *anti*-indacenodibenzothiophenes. **S. Durham**, C.K. Frederickson, J. Marshall, M.M. Haley

CHED **1406.** 1,3-Dipolar cycloadditions to 1,4-quinones. **C. Wasacz**, W. McMahon

CHED **1407.** Synthesis and evaluation of peptides for RNA world hypothesis. **M.Z. Jorge**, R. Patel, K. Sweeney, U. Muller, J.G. Schellinger

CHED **1408.** Analysis of pyrrolizidine alkaloids in *Cryptantha maritima*. **C.R. Barton**, **M.M. Lease**, **M.E. Hillman**, **J.D. Jacobs**, **O.E. Starks**, **R.B. Kelley**

CHED **1409.** Synthesis of naphthalene diimides with varying core substitutions for use in donor acceptor aromatic interactions. **M. Stern**, J.J. Reczek

CHED **1410.** Development of a novel aldehyde C-H bond functionalization reaction using an organocatalytic methods for the nucleo-acylation of alkenes. **N.P. Biewer**, K. McMahon

CHED **1411.** Studies of xenocoumacin-1-benzylideneacetone Michael adduct formation. **C. DeShambo**, M. VanMieghem, M. Cherney, A. Koopmann, K.A. Bichler, S. Forst, J. McGraw

CHED **1412.** Rapid synthesis of *N*-methyl-*N*-(3-trifluoromethylbenzyl) formamide. **T.A. Dostert-Azzarello**, L.I. Bobyleva, M.M. Bobylev

CHED **1413.** Photochemical reactivity profiles of quinoxalenediyne isomers. **S.A. Valenzuela**, B.F. Gherman, J.D. Spence

CHED **1414.** Synthesis of (-)-duryne and homologues. **T. Schempp**, D.B. Ball

CHED **1415.** Tailor-made GNRs: Controlled conversion of polydiacetylenes into graphene nanoribbons. **R. Mccurdy**, R. Jordan, S. Khan, Y.F. Rubin

CHED **1416.** Rapid synthesis of *N*-(2-chlorobenzyl)-*N*-methylformamide. **E.Y. Mojica**, L.I. Bobyleva, M.M. Bobylev

CHED **1417.** Rapid synthesis of *N*-methyl-*N*-(2-naphthylmethyl)formamide. **B. Hatfield**, L.I. Bobyleva, M.M. Bobylev

CHED **1418.** Synthesis of a degradation product of benzobicyclon. **C. Park**, **J. Kalbfleisch**, L. Rubottom, J.J. Gladfelder, D.B. Ball

CHED **1419.** Progress towards the synthesis of a desmethyl englerin A analog. **E.B. Pimentel**, M. Andrus, D. Wilcox

CHED **1420.** Visible-light-promoted formation of α-tertiary amines via a N-centered radical approach. **C.E. Keating**, M.M. Tierney, A.A. Lamar

CHED **1421.** Preparation of diliginol model compounds. **K. Zhang**, J. Pence, R. Lamb, Y. Zhu

CHED **1422.** Tandem Ugi-Smiles Diels-Alder reactions: Evaluation of substrate scope. **A. Fox**, S. Luesse

CHED **1423.** Synthesis of 6- and 7-(4-aryl)-*N*-*acetylglyoxylamides*. **M. Covington**, L. Desrochers, N. Kumar, D. Black, **T.E. Goodwin**

CHED **1424.** Towards a chlorin-based fluorophore synthesis for pharmacokinetic diagnosis in neglected tropical diseases. **S.M. Bridges**, G.R. Naumiec

CHED **1425.** Chemical synthesis of the cyclic peptide stylissamide X, a cell migration inhibitor. **K. Warrick**, J. Chaytor

CHED **1426.** Dialkyltriazene decomposition leading to bromoarenes: A boron tribromide-mediated process. **V. Kuipers**, A.L. Korich

CHED **1427.** Stereoselective synthesis of fluorinated β-lactams and β-aminoesters. **A.C. Sigler**, J.C. Easdon

CHED **1428.** Sulfonated maleimides: New monomers for thermally robust polymers. **J. Linville**, A.L. Korich

CHED **1429.** Total synthesis of a series of ^{13}C-labeled isotopomers of xanthohumol: The primary prenylated chalcone in the inflorescence of hops plants. **D. Ellinwood**, P.R. Blakemore

CHED **1430.** Formation of trisubstituted naphthalenes: Development of a new benzannulation strategy. **P. Mansour**, A.L. Korich

CHED **1431.** Preparation of keto sulfoxonium ylides from carboxylic acids. **A. Krahn**, M. Paeth, R. Enright, P. Willoughby

CHED **1432.** Synthesis of small-molecule inhibitors of botulinum neurotoxin. **K. Recabo**, **E. Slick**, S.M. Ensel

CHED **1433.** Novel synthesis of ferrocenyl epoxides derivatives to explore their biological potential as anticancer and antioxidant compounds. **J. Davila**, I. Montes-González, J.C. Aponte-Santini

CHED **1434.** Bisphosphorylimides as organocatalysts for asymmetric Friedel–Crafts reactions. R.G. Iafe, **L. Ahlberg**, **C. Thompson**, G. Diaz, B. Klasic

CHED **1435.** Synthesis of linker molecules connect nanomaterials for solar PV cells. **D. Melchor**, X. Herrera, E. Juette, J. Zhang

CHED **1436.** *N*-Propylmaleamic Acid (NPMA): Concentration dependent chemical shift variability of vinyl protons. **L. Pilarz**, W.A. Price

CHED **1437.** Synthesis of amino acid radical precursors. K.N. Carter, **C.M. Foscue**

CHED **1438.** Total synthesis of cladosin C. **J. Mease**, H. Burdge, K.P. Reber

CHED **1439.** Synthetic studies on squamostanin C. **Y. Hu**, **P.J. Miller**, K.J. Quinn

CHED **1440.** Total synthesis and biological evaluation of tryptamide derivatives. **Z. Shen**, E.K. Leggans

CHED **1441.** Exploration of α-glucosidase inhibitors via synthesis of C-linked β-D-glucose analogs. **B. Pero**, J. Chaytor

CHED **1442.** Progress toward the synthesis of guignardianone E. **S. Lewis**, C.J. Nichols

CHED **1443.** Comparing transverse relaxation (T_2) times between low and high field NMR's for reaction of chlorosulfonyl isocyanate with alkenes. **Z. Beavis**, **S. Van Horne**, D.F. Shellhamer

CHED **1444.** Efforts toward the total synthesis of (+)-bovidic acid. **A.B. Millham**, K. Nicastri, K.J. Quinn

CHED **1445.** Relationship between biaryl ligand structure and reactivity in under-air direct arylation. **J. McAfee**, J. Fritz

CHED **1446.** Aldol reactions: A lab aimed at second semester organic chemistry. **J. Burroughs**, R.V. Macri

CHED **1447.** Measuring the cell death of novel indolyl amines. **B. Lowder**, T. Bishop, M. Dosso, T. Tolentino, C.R. Whitlock

CHED **1448.** Rapid synthesis of *N*-(4-bromobenzyl)-*N*-methylformamide. **H. Lee**, L.I. Bobyleva, M.M. Bobylev

CHED **1449.** Rapid synthesis of *N*-(3-chlorobenzyl)-*N*-methylformamide. **T.A. Skinner**, L.I. Bobyleva, M.M. Bobylev

CHED **1450.** Investigation of potential coformers for synthesis of sulfa drug cocrystals. **A. DeMaet**, D. Adsmond

CHED **1451.** Progress toward the total synthesis of (+)-cryptofolione and development of natural product analogues. **K. Nicastri**, C.N. Ndi, J. Torres, P.R. Hanson

CHED **1452.** Introverted bis-Au cavitands: Cavity-dependent catalysis. **L. Digal**, M.P. Schramm, T. Iwasawa

CHED **1453.** Search for resonance in vinylsilyl anions: Synthesis of silyl substituted 9-methylenefluorene. **C. Fowler**, E. Gulotty, W.R. Winchester

CHED **1454.** Synthesis and study of a vinylsilole. **J. Robertson**, C. Duke, W.R. Winchester

CHED **1455.** Design and synthesis of new ternary cocrystals using carboxyphenols. **P. Sperstad**, D. Adsmond

CHED **1456.** Investigating analogs of eflornithine, an irreversible inhibitor of ornithine decarboxylase. **L. Oxtoby**, L. Liu, N. Gerstner, J.M. Schomaker

CHED **1457.** Synthesis of 2-substituted quinoline-4-carboxylic acids from 5- and 7-fluoroisatins and benzylideneacetones via the Pfitzinger reaction. **A. Imanishimwe**, L. Desrochers, T.E. Goodwin

CHED **1458.** Synthesis of 2-substituted, 3-methylquinoline-4-carboxylic acids from 5- and 6-bromo-, chloro- and fluoro-isatins via the Pfitzinger reaction. **A. Shuler**, L. Desrochers, T.E. Goodwin

CHED **1459.** Intermolecular halogen bonding and non-conventional hydrogen bonding in arylene ethynylene oligomers. **Z. Kehoe**, G. Woller, E. Bosch, N.P. Bowling

CHED **1460.** Electrophilic alkylations in aqueous-surfactant solutions. **Z. Gregg**, E. Ballard

CHED **1461.** New approaches to the synthesis of N-heterocyclic carbenes. **G. Schlicht**, M.O. Odago

CHED **1462.** Synthesis of 2-cycloheptatrienyl iminodioic acid, a potential switchable organic linker for Metal Organic Frameworks (MOFs). **A.R. Satterfield**, B. Meeker, D. Jackson, R.W. Morrison

CHED **1463.** Synthesis and reactions of some 1,2-diacyldiaziridines. S.M. Bonser, **I. Jacome Ottati**

CHED **1464.** Utilization of nucleobase interactions to develop energy and electron transfer systems. **H.M. Owens**, C.M. Lawrence

CHED **1465.** Thermodynamic and structural impact of α,α-dialkylated residue incorporation in a β-hairpin peptide. **S. Schettler**, G.A. Lengyel, G.D. Gette

CHED **1466.** Synthetic strategies towards the synthesis of guanacastepene A. **M. Shinn**, T.V. Ovaska

CHED **1467.** Withdrawn.

CHED **1468.** Research–derived experiments for the undergraduate teaching laboratory. D.G. Hamilton, **S.E. Carter**

CHED **1469.** Synthesis of a photolabile derivative of T-0632 to study GLP-1R. **S. Eslami**, G. Towers, D.R. Haines

CHED **1470.** Exploring the edge-modification of graphene. **P.N. Rudd**, J. Reczek

CHED **1471.** Synthesis of 1,3,4-oxadiazoles using dibromotriphenylphosphorane. **E. Bliss**, K. Merringer, E. Peters, **B. Sowers**, R.E. Grote

CHED **1472.** Synthetic studies toward 2-bromo-4,5-dimethylanilline en route to hunanamycin A. **G.J. Baldree**, S.M. Kennedy

CHED **1473.** Evaluation of imines as cation sensors in water samples. **M. Seidel**, **N. Rosenfeld**, A. Gaynor, J. Bennett

CHED **1474.** Estimating imine basicity trends by multinuclear NMR. **N. Capra**, J. Bennett

CHED **1475.** Introduction of MOM and MEM protecting groups via acid-catalyzed transacetalization using solid acid catalyst. **J.M. Edgecomb**, **K.G. Fosnacht**, G.L. Milligan

CHED **1476.** Synthesis of *bis-3,4-(2'-acetoxybenzoyl) furoxan*. **A.A. Richards**, N.M. Wachter

CHED **1477.** Advancing organic chemistry laboratory techniques using the open source arduino platform. **D.M. Lutz**, **C. Konow**, C.E. Stilts

CHED **1478.** Dioxane-mediated *N-formylation*. **B. King**, A.G. Wenzel

CHED **1479.** Withdrawn.

CHED **1480.** Synthesis and NMR characterization of new bromopyridine thiosemicarbazone compounds. **J.T. Kimrey**, E.C. Lisic

CHED **1481.** Calculation of extinction coefficients for meso-substituted porphyrins in different solvents. **A. Novaj**, S.N. Khayyo, P.K. Kerrigan, J. Batarseh, S. Maio, R. Guglielmo

CHED **1482.** Peripheral functionalization of AzaBODIPY for 2D and 3D assemblies. **D. McKinzey**, F. D'Souza, S. Shao

CHED **1483.** Synthesis and reactions of dicyanopyrazines. A.T. McGrath, **A.M. Schoffstall**

CHED **1484.** Approach to the synthesis of new isatin-linked chalcones. **D. Wade**, L. Desrochers, T.E. Goodwin

CHED **1485.** Relative reactivity of a series of SNC-Rh(I) and Ir(I) pincer complexes in catalytic transfer hydrogenation and arene borylation. **K. Barko**, P.L. Osburn

CHED **1486.** Synthesis of sulfonamides utilizing green, one-pot methods. **B. Tomiczek**, J.K. Vohs

CHED **1487.** Searching for chemical signals in orang-utans (*Pongo spp.)*. **P. Ravikumar**, A. Umuhire-Juru, S.B. Bradley, G. Banes, T.E. Goodwin

CHED **1488.** Exploring the utility of halogen bonding in the creation of abiotic helices. **A. Schneider**, E. Bosch, N.P. Bowling

CHED **1489.** Synthesis of photolabile T-0632 derivatives to aid GLP-1R active site exploration. **L. Bancroft**, D.R. Haines

CHED **1490.** Synthesis of 2-substituted quinoline-4-carboxylic acids from 5- and 6-bromo-, chloro-, and iodo-isatins via the Pfitzinger reaction. **G. Stanton**, L. Desrochers, T.E. Goodwin

CHED **1491.** Intramolecular halogen bonding of 2,1,3-benzothiadiazole containing molecules. **L. Mancheski**, S. Giebel, E.D. Speetzen, E. Bosch, N.P. Bowling

CHED **1492.** Progress toward the synthesis of the heterocycle Choi. **J.M. Spehar**, M.S. Leonard

CHED **1493.** Isolation of novel compounds from *Garcinia binucao* via enzymatic extraction. **M. Lesko**, K.M. Halligan

CHED **1494.** Chemoselective hydrodehalogenation and deuterodehalogenation of aryl halides using borohydrides and supported metal catalysts. **J. Garcia**, D.B. Cordes

CHED **1495.** Synthesis of 2-substituted quinoline-4-carboxylic acids from 5- and 7-fluoroisatin via the Pfitzinger reaction. **D. Shah**, M. Abdulrahim, L. Desrochers, T.E. Goodwin

CHED **1496.** Microwave synthesis of β-fluoroamides from alkenes. **A. Trimble**, M.L. Druelinger

CHED **1497.** Effects of solvents on the iron-catalyzed N-demethylation of opiate alkaloids. **B. Evangelisti**, K.M. Halligan

CHED **1498.** Discovery of a novel mechanism for cyclopropyl ring opening. **G.W. Larson**, J.T. Ippoliti

CHED **1499.** Two-step synthesis of flavonoids using task-specific ionic liquids. R.N. Manchanayakage, **R. Potenzino**

CHED **1500.** Effects of alkyl chain length on carbohydrate organogel formation and properties. **N. Toupin**, J. Chaytor

CHED **1501.** Transesterification of hypophosphorous esters: A methodology study. **A.V. Carmona**, N. Neris, S. Deprele

CHED **1502.** Synthesis of an ethylene-linked calixarene dicavitand scaffold for dimeric Template-Assembled Synthetic Proteins (TASPs). **E.J. Peterson**, N.A. Yakelis, J. Freeman

CHED **1503.** Preparation of biocompatible nanoparticle aggregates. **A. Taylan**, A.G. Wenzel, J.M. Berlin

CHED **1504.** Organocatalytic hydroamination reactions of dienes. **S. Srivastava**, A.G. Wenzel

CHED **1505.** Synthesis of indolylmalonamides and analysis of their metal binding properties. **M. Frame**, J. Jennings, A.K. Franz

CHED **1506.** Synthesis of octavalent dendrimers for glycosylation. **J. Cerney**, K.D. McReynolds

CHED **1507.** Synthesis of small functionalized molecules using copper-catalyzed Atom Transfer Radical Addition (ATRA). **M. Baldwin**, T. Pintauer, S. Fischer

CHED **1508.** Nickel-catalyzed borylation of aryl *O-sulfamates*. **K.R. Holman**, P. Burree, J. Edmondson, K. Hill, A.L. Silberstein

CHED **1509.** Synthesis of cellobiose and lactose terminated glycodendrimers. **L. Gwarada**, K.D. McReynolds

CHED **1510.** Modified click-style Sonogashira coupling reactions involving silyl-protected alkynes. **M.J. Mio**, K.M. Barbour, R. Beltman, Y.M. Brikho, N.R. Boynton, N.H. Husseini, M.M. Payne, B.M. Ross, K.M. Suiter

CHED **1511.** Synthesis of a novel chiral ferrocene ligand. **B. Davies**, C. Denler, J. Sturdevant, N.E. Carpenter

CHED **1512.** Synthesis of ferrocenyl-substituted N-heterocyclic carbenes. **D. Saugar**, M.O. Odago

CHED **1513.** Design, synthesis and biological evaluation of berberine analogs as anticancer agents for triple negative breast cancer. **D. Bradford**, F.L. Payton

CHED **1514.** Synthesis of N-(N'-(3-propyl)-N"-methylimidazole-2-thione) diethylenetriamine tetraacetic acid for the reduction of nuclear waste. **R.K. Pontius**, M.M. Sibley, M. Wetzler

CHED **1515.** Synthesis and electrochemistry of pyrazinium salts. **N. Wagner**, M. Worke, **C. McCauley**, V.A. Sichula

CHED **1516.** Design, synthesis, and biological evaluation of berberine analog as an anticancer agent. **N. Tran**, F.L. Payton

CHED **1517.** Investigation of substituted furaldehydes in the Passerini-Smiles reaction. **W. Friederich**, C. Summers, S. Luesse

CHED **1518.** Facile synthesis of resveratrol analogues and inducing osteogenesis in mesenchymal stem cells. **L. Daley**, E. Barth, G. Cabezas, D. Paull

CHED **1519.** Investigation of catalysts and conditions for the synthesis of hindered imines and application to the preparation of the camphor imines of hindered substituted benzylamines. S.A. Corlett, **I.F. Germek**

CHED **1520.** Chasing a universal method for the mono-substitution of symmetrical diols. **L. Daley**, D. Paull

CHED **1521.** Facile ring opening of cyclic ethers using sodium borohydride and iodine. **A. Ramayani**, **M. Cummings**, M. Nigam, P. Dhar

CHED **1522.** Approaches to molecular interlocking in the solid state. D.G. Hamilton, **D. Sibai**

CHED **1523.** Synthesis and electrochemical properties of a homologous series of cyanine-type and anthracenyl compounds with thienyl moieties. **N.B. Burman**, J.G. Rowley

CHED **1524.** Synthesis of furan derivatives and the kinetics of their Diels-Alder reactions with *N-(4-fluorophenyl) maleimide*. **T.R. Jones**, W. Hollis, P.A. Deck

CHED **1525.** Magnetic anisotropy of *C-nitroso compounds*. **C.E. Owens**, S.C. Blackstock, A. Kelley

CHED **1526.** New triphenylamine derivatives for use in nondoped organic light emitting diodes. **A. Dahl**, V.A. Sichula

CHED **1527.** Synthesis of novel paraben derivatives. **M. Bache**, S. Merrill, K. Pate

CHED **1528.** Development of an enantioselective allenoate claisen rearrangement. **I. Laufer**, A.G. Wenzel

CHED **1529.** Preliminary characterization of fossilized plant exudates by ^{13}C nuclear magnetic resonance spectroscopy. **T.V. Nguyen**, J.B. Lambert

CHED **1530.** Synthesis of a novel chiral anthracene-based ligand for incorporation in supramolecular assemblies. **A. Stamoulis**, R.M. Triano, K.N. Raymond

CHED **1531.** Steric and catalytic effects of alcohols on the transamination of naphthalimides. **T.N. Kysely**, **B.A. Smith**, D.E. Lewis

CHED **1532.** Amide formation studies en route to Hunanamycin A. **S.K. Gillis**, **J.E. Thames**, S.M. Kennedy

CHED **1533.** Green synthesis of novel fluorescent, photochromic, and thermochromic imines and diimines. **W. Evans**, J. Bennett

CHED **1534.** Green synthesis of substituted benzoin analogs and qualitative analysis with redox indicators for organic chemistry laboratory. **G. Chesser**, J. Bennett

CHED **1535.** Structure determination of a family of bioactive lipids isolated from the larvae of the Argentine cactus moth, *Cactoblastis cactorum*. **D. Cervasio**, **T. Schwertfeger**, T. Potter, M. Todd, F.M. Rossi

CHED **1536.** Facile synthesis of benzo-fused sulfur-containing heterocycles. **S. Alam**, F. Robertson

CHED **1537.** Complete synthesis of *S–(+/-)–lycoperdic acid*. **J. Singh**, R.W. Denton

CHED **1538.** Synthesis of new precursors to the pyramidalized alkene pentacyclo[4.3.0.$0^{2,4}$.$0^{3,8}$.$0^{5,7}$]non-4-ene (2). **C. Stow**, R. Kontos, M.A. Forman

CHED **1539.** Intramolecular hydroamination of unfunctionalized alkenes in the presence of gold catalysts. **M.M. Zendali**, A.G. Wenzel

CHED **1540.** Progress towards the synthesis of a Baeyer-Villiger enzyme mimic. **M. Khan**, F. Robertson

CHED **1541.** Structural determination in donor-acceptor columnar liquid crystals series. **M. Hill**, J. Reczek

CHED **1542.** Toward spin bearing polymers as components of spintronic systems. **K. Sai**, **W. Guan**, **R. Mac**, **Y. Chen**, T.F. Hom, D.J. Brook

CHED **1543.** Towards the synthesis of Stachybotrin D. **S. Coody**, D.C. Bromfield-Lee

CHED **1544.** Studies en route to altersolanol derivatives. S.M. Kennedy, **T.C. Bentzel**, **B.L. Frey**

CHED **1545.** Chasing enantioselectivity: Synthesis of chiral α-quaternary carboxylic acid building blocks. **E. Barth**, D. Paull

CHED **1546.** 6-Gingerol extraction, isolation, and reduction to 6-gingerdiols. **C.D. White**, E. McGuffie, T. Harris, J.J. Krikke, D.G. Kovacs

CHED **1547.** Oxadiazole based liquid crystals: Phase behavior and efforts to improve the synthetic route to the target compounds. **G. Reyes**, E. Scharrer

CHED **1548.** Synthesis of indole derivatives and 1,2-aminoalcohols via *N*-tosyl 2-alkenylaniline oxides. **L.N. Hines**, C.J. Monceaux, C. Tutwiler

CHED **1549.** Has anybody seen my gal? Ready access to lincosamide analogs from diacetone galactose. **C. Love**, Z. Cannone, J. Portelinha, A.M. Angeles Boza, M. Peczuh

CHED **1550.** Colorimetric studies of isoniazid-based anion sensors. **J. Warner**, M.O. Odago

CHED **1551.** Synthesis of a new molecule, 2,3-Butanedione Tertbutyl-Thiosemicarbazone (BDMO-tBTSC) and characterization by a new 500 MHz nuclear magnetic resonance spectrometer. **H.M. McFadden**, A. Susnjar, E.C. Lisic

CHED **1552.** Synthesis of fatty acid polyamides. **E. Corral**, **J. Arriaga**, **R. Kim**, **A. Keshishian**, A. Oganesyan

CHED **1553.** Synthesis and characterization of D-glucosamine derived lipids as low molecular weight gelators. **P. Kozlowski**, J. Morris, A. Chen, G. Wang

CHED **1554.** Synthesis and purification of glycodendrimers. **U. Farah**, K.D. McReynolds

CHED **1555.** Synthesis and characterization of ferrocenyl curcumin analogues as potential antioxidant and antibacterial compounds. **X. Santiago-Maldonado**, J. Rivera, I. Montes

CHED **1556.** UV/Visable spectra and the solvatochromic properties of various 2,6- diaryl-*3H-imidazo[4,5-d]pyridines*. **J. Orlandi**, J.K. Murray, M.J. Castaldi, M. Bauman

CHED **1557.** Synthesis of polyhydroxylated indolizidine using ruthenium catalyzed dihydroxylation reaction. **C. Giannetti**, L.J. Liotta

‡ *Cooperative Cosponsorship*

CHED **1558.** Synthesis of acetylenic and pyridyl bicyclobutanes. **G. Giardino**, L.J. Tilley

CHED **1559.** Lowering the catalyst loading in cobalt-catalyzed Kumada couplings. **S.D. Chafin**, **K.P. Zachariah**, M.C. Perry

CHED **1560.** Synthesis of a novel N-hetrocyclic carbene ligand for the use of enantioselective catalysis. **M. Licata**, P.J. Lombardi

CHED **1561.** Synthesis and properties of triazine based dendrimers constructed using hydrazine linkers. **A.V. Ananin**, M.B. Steffensen

CHED **1562.** Investigation of regioselective and stereoselective additions to (1R)-(-)-nopol, a bicyclic sterically hindered alkene. **D. Joaquin-Castaneda**, K.C. Sorensen-Stowell

CHED **1563.** Reactions of 6-oxoverdazyls for use as spin probes. A. Herrera, T. Pan, **D.J. Brook**

CHED **1564.** Kinetic study of reactivity of *para*-substituted iodo-phenylalkynes in the copper (I)-catalyzed azide-alkyne cycloaddition reaction. **H. Rossiter**, A. Nazarova, V. Fokin

CHED **1565.** Synthesis of UIO-67 derivatives for site-isolated reactions. **C.E. Lemmon**, **S.A. Larson**, M.C. Perry, L.G. Beauvais

CHED **1566.** Synthesis of methoxy-tetrahedrane by coupling and elimination of dibromosilylcylcobutane. **E. Hickey**, L.J. Tilley

CHED **1567.** Synthesis of water-soluble tetrasulfonated calix[4]arenes with a reactive methylene-bridge substituent. **J.D. Sundberg**, J.L. Fantini

CHED **1568.** Concise synthesis of COX inhibitor BRL-37959. **D. Hinz**, S. Ahmed, M. Hossain

CHED **1569.** Synthesis of novel oxazolidinone anitbacterials. **J.K. Bardwell**, **T.J. Higgins**, C.T. Ippoliti, **E.J. Keil**, **T.J. Ogorek**, A.M. Heuer, J.T. Ippoliti

CHED **1570.** Copper(I)-catalyzed silylations using disilanes. **B. Thomas**, B. McCarty, R. Van Hoveln

CHED **1571.** Protection of primary amines with high molecular weight silanes. **A. Pancoast**, M.T. Wentzel

CHED **1572.** How do ether and amine bridges affect the conjugation in monomacrocyclic dendrimers? **A. Smyly**, B. Nash, D.H. Magers, S.A. Smith

CHED **1573.** Synthesis of esters and amides using both flow and microwave reactors. **E. Peters**, M.T. Wentzel

CHED **1574.** Progress towards the synthesis and chemistry of some novel diaziridines. S.M. Bonser, **J.F. Urena**

CHED **1575.** Evaluating the impact of tether position on the intramolecular oxazolium salt/azomethine ylide cycloaddition sequence. **S.E. Rourk**, D.L. Warner

CHED **1576.** Three-component coupling of an arylboronic acid, aryl halogen and ketene to form benzyl phenyl ketone derivatives. **P.A. Shelton**, B. Martin, E. Fussell

CHED **1577.** Pyridine derivatives as sources of nucleophilic fluorine. B. Maki, **S. Marrujo**

CHED **1578.** Synthesis of all-trans cyclobutyl systems and investigation of electron-withdrawing substituents. **M.S. Wolf**, L.J. Tilley

CHED **1579.** Synthesis and optimization of a new synthetic route to modified thymidine monomers. **M. Magnuson**, M.P. Maddox

CHED **1580.** Factors determining the Wagner-Jauregg reaction. **S. Johnson**, S. Tartakoff

CHED **1581.** Progress toward the synthesis of pyrrole-based alkaloid natural products. B. Maki, **A. Garcia**

CHED **1582.** Mercury-free hydration of terminal alkynes. **P.A. Shelton**, B. Ide, J. Thompson, S. Sulcer

CHED **1583.** Investigation of the formation of an imine between an aldehyde with a conjugated pi bond and a primary amine. **H. Hobbs**, K.C. Sorensen-Stowell

CHED **1584.** Synthesis and evaluation of phenylglycine-derived amino-oxazolines as anti-oxidants. B. Maki, **Y. Xiu**

CHED **1585.** Surfactant synthesis of hypophosphite esters involving phosphorus chemistry. **A. Gonzalez**, S. Deprele, **V. Lee**

CHED **1586.** Synthesis of [2.1.2]-bicyclic heterocycles inspired by Lycojaponicumin natural products. B. Maki, **J. Alcon**

CHED **1587.** Comparison of iodination methods on aryl heterocycles: The curious synthesis of 2,3,4-triiodo-5-methylthiophene. **N. LeValley**, J.B. Benedict, D.G. Patel

CHED **1588.** Microwave-assisted general synthesis of highly-substituted anthraquinone derivatives. **A. Delahunty**, J.J. Reczek

CHED **1589.** Synthesis and phase behavior of new oxadiazole-based liquid crystals possessing multiple lateral groups. **R. Grate**, E. Scharrer

CHED **1590.** Three component separation of an unknown sample in order to refresh student techniques before organic II laboratory. **P.A. Shelton**, S. Belton, J. Crews

CHED **1591.** Far-red emitting squaraine dye: Synthesis, optical properties, and cyanide sensing. **M.A. Valencia**, T. Liu, X. Liu, K.D. Belfield

CHED **1592.** Isoxazole-based inhibitors of the neuraminidase enzyme of the influenza virus. **P. Rahman**, J. Singh, R.W. Denton, A. Glanzer

CHED **1593.** Synthesis and characterization of 5-(3'-thienyl)-1-mercaptopentane capped lead sulfide nanoparticles for polymeric photovoltaic cells. **S.W. Steele**, M.J. Strauss, J. Zemke, R.W. Kopitzke

CHED **1594.** Benzylic amide synthesis using a heterogeneous catalyzed continuous flow reactor. M.T. Wentzel, **J. Scheeler**

CHED **1595.** Fluorination of 2-hydroxybenzyl alcohol. **S. Hernandez**, R.E. Rosenberg

CHED **1596.** Alteration of HMBC parameters to show $^{4}J_{H\text{-}C}$ *and* $^{5}J_{H\text{-}C}$ correlations for the structural elucidation of a fungal secondary metabolite. **E.J. Sperry**, A. Jordan

CHED **1597.** Better way to synthesize ketones. L. Farber, **S. Baer**, **S. Zupetz**, **M. Filja**

CHED **1598.** Tetra-*meso*-substituted porphyrins *via* mechanochemistry: Reaction homology and applications of a porous catalyst. **Q. Su**, T.D. Hamilton

CHED **1599.** Pre-monomer peptidomimetic synthesis using thiol-ene click chemistry. **X. Liu**, L. Witus

CHED **1600.** Regioselective ring opening of phenyl aziridines. **A.J. Wong**, J.A. Tarahomi, M.E. Hart

CHED **1601.** Synthesis of thiol and carboxylate ligands for nanocrystals in luminescent solar concentrators. **E. Woodward**, R.C. Chambers

CHED **1602.** Solid-state chemistry of dimers of reactive nitrile oxides. **S. Whitcomb**, W.H. Ojala

CHED **1603.** ^{13}C Kinetic isotope effects and the mechanism of the Cope-type hydroamination of alkynes. **R. Rivera**, D. Singleton, Y. Nieves-Quinones

CHED **1604.** Equilibrium constants in the Diels-Alder reactions of furan derivatives with *N*-(4-fluorophenyl) maleimide. W. Hollis, **D. Stum**, P.A. Deck

CHED **1605.** Comparison of new isatin thiosemicarbazone derivatives: NMR structure determination. **A. Susnjar**, H.M. McFadden, E.C. Lisic

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Physical Chemistry

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N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1606.** New method for measuring acidity in methanol. **C.G. Lamunu**, **E.D. Lorance**

CHED **1607.** Measuring adsorption phenomena using femtoliter arrays. G.M. Nishioka, **K.S. Huggler**, T.N. Dao, C.W. Sokolik

CHED **1608.** Doping of a thermotropic liquid crystal with ferromagnetic platelets. **M. Van Winkle**, A. de la Cotte, A.G. Yodh

CHED **1609.** Barriers to bond rotation in *N,N-dimethylbenzamides probed using temperature dependent ^{1}H-NMR spectroscopy*. W.T. Grubbs, **M. Ma**

CHED **1610.** Determination of acid and base effects on the surface chemistry of silver nanoparticles. **P. Kraj**, M.K. Parker, J.D. Mimbs, R. Vaithi, C.S. Seney

CHED **1611.** Polyphosphate mediation in synthesis of doped alloy semiconductor nanoparticles. **P. Kraj**, D. Moore

CHED **1612.** GC/QQQ limits of detection for biomolecules in abiotic aerosols. **M.C. Roach**, T.M. Christensen, J. Sebree

CHED **1613.** Survey of proline conformational behavior in protonated gas-phase XxxProGlyGly. **A.E. Glass**, K.A. Dickerson, D.A. Hales, T.J. El-Baba, D.E. Clemmer

CHED **1614.** Synthesis of biofunctionalized self-assembled monolayers on zinc selenide. **A. Merrill**, A.R. Noble

CHED **1615.** Fluorescence studies on a series of carboxylic acid dyes. **R. Ashmore**, M. Elioff

CHED **1616.** Analysis of the quantum yield and photodegradation of anthraquinone-based dyes. **M. Thomas**, S.J. Sobeck

CHED **1617.** Coupling reactions catalyzed by palladium nanoparticle/carbon microsphere composites. **S. Murphy**, K.M. Metz

CHED **1618.** Synthesis and characterization of lipid-coated nanoparticles as drug delivery vehicles. **C. Munjar**, B.D. Gilbert

CHED **1619.** Plasma-assisted atomic layer deposition of GeS_2 thin films from $GeCl_4$ and H_2S precursors in a student designed PAALD chamber. **B. Poulter**, M. Gonzalez, R. Rodriguez

CHED **1620.** Millisecond enzyme kinetics in picoliter volumes. **R. Law**, J. Nguyen, T. George, P. Abbyad

CHED **1621.** Underpotential deposition of nickel on electrodeposited p-type Cu_2O films and its effects on photocatalytic activities and stability of p-type Cu_2O films. **N. Budin**, **S. Hilston**, A. Fillinger

CHED **1622.** Hyperfine analysis and global fitting of near-infrared electronic spectra of AuS. **A. Parsons**, **S. Gleason**, T.D. Varberg

CHED **1623.** Properties of antioxidant deep eutectic solvents. **D. Jones**, J.C. Goeltz

CHED **1624.** Mixed self-assembled monolayers formed through the coadsorption of decylthiocyanate and octanethiol on Au(III) surfaces. **R. Giinther**, A.F. Raigoza

CHED **1625.** Characterization of single-walled carbon nanotube-porphyrin complexes with different metal centers. R. Selzer, **R. Polvere**

CHED **1626.** Using ATR-IR spectroscopy to study heterogeneous catalysts. **E. Christoffersen**, J. Lindale, D.G. Kovacs

CHED **1627.** Gas-phase measurement of the barrier to *cis*-trans interconversion of proline in a tetrapeptide. **K.A. Dickerson**, A.E. Glass, D.A. Hales, T.J. El-Baba, D.E. Clemmer

CHED **1628.** Determination of the limiting equivalent conductivity and thermodynamic equilibrium constant for the formation of $LaCl^{2+}$ ion-pairs at 25 °C using lanthanum chloride/sodium chloride mixtures. **B. Durante**, G.H. Zimmerman

CHED **1629.** Synthesis and photophysics of lanthanide/transition metal heterobimetallic complexes. **K. Burke**, C. Heaney, A. Hill

CHED **1630.** Tracking ultraviolet degradation of *p*-aminobenzoic acid and two derivatives. **G.F. Jocas**, S.J. Sobeck

CHED **1631.** Solvent mediation of unimolecular helical exchange dynamics in the synthetic helical peptide Z-Aib_6-β-Ala-OMe. **C. Foster-Spence**, M.C. Rotondaro, J. Dickovick, M.A. Kubasik

CHED **1632.** Fundamental structural studies of thiolate-protected gold clusters using Raman spectroscopy. **L. Tsang**, N. Hammer

CHED **1633.** Withdrawn.

CHED **1634.** Drugs and light: Predicting the photosensitivity of tolbutamide and sulfisoxazole using the change in dipole moment by Stokes shift analysis. **A. Costley**, A. Bills

CHED **1635.** Characterization of the *N^6-methyl-formamidopyrimidine lesion*. **H. Pan**, S.N. Bamberger, R.S. Bowen, C.K. Malik, T.L. Johnson-Salyard, C.J. Rizzo, M.P. Stone

CHED **1636.** Microfluidic vibrational strong coupling of organometallic complexes in aqueous solutions. **S.R. Casey**, J.R. Sparks

CHED **1637.** Study on the effect of salt concentration on the adsorption and rupture of phospholipid vesicles on a silicon dioxide surface. **A. Krone**, I. Alhallak, P.J. Kett

CHED **1638.** Detection of trace amounts of NO_2 using CW-CRDS. **J. Kozubal**, J.B. Dudek

CHED **1639.** Investigating the photophysical properties of indolizine-squaraines. **R. Nelson**, L.E. McNamara, T. Rill, A. Huckaba, N. Hammer, J.H. Delcamp

CHED **1640.** Quantification of binary solution non-ideality through temperature dependent measurements of viscosity, molar volume, and refractive index of mixtures of hexane/hexan-1-ol and anisole/methanol. **H.S. Slocumb**, C.K. Kalcic, S.A. Price, G.R. Van Hecke

CHED **1641.** Systematic binary isobaric solid-liquid phase diagrams of straight-chained carboxylic acids. **C.M. Adams**, G.R. Van Hecke

CHED **1642.** Ring opening metathesis polymerization of a ciprofloxacin-conjugated copolymer for pulmonary intracellular antibiotic delivery. **N. Warner**, M. Zhao, D.M. Ratner, D.J. O'Leary

CHED **1643.** Synthesis and characterization of silver triangular nanoprisms. **M. Bruening**, L. Peng, R.P. Van Duyne

CHED **1644.** Synthesis and characterization of lipid and silver coated gold nanoparticles with pMBA tags. **A.B. Smith**, B.D. Gilbert

CHED **1645.** Spectroelectrochemical behavior of electrodeposited Zn on indium tin oxide surfaces and modeling of nanoparticle aggregation via Maxwell-Garnett theory. **C.M. Schneps**, J.S. Kegerreis, J.N. Richardson

CHED **1646.** Thermodynamic effects of pendent chain length in the agregation of perylene diimide derivatives. X. Xu, **J.M. Szarko**

CHED **1647.** Spectroscopic and computational studies of the hydrogen bonding interactions of hydroxyethyl ethers. **A. Williams**, J.T. Kelly, N. Hammer, S.R. Davis

CHED **1648.** Stable isotope chemistry in Titan haze aerosol. **A. Wold**, T. Gautier, J. Stern, J. Sebree, M. Trainer

CHED **1649.** Synthesis and characterization of gadolinium-silica precipitation tubes. **C. Sabal**, D.P. Weller, J.J. Pagano

CHED **1650.** Temperature and electric field dependence of asymmetric stretching of nitrate ion. **K. Jones**, M.J. Nee

CHED **1651.** Phase transitions of barium hydrogen phosphate, a ferroelectric material, characterized by nuclear spin-lattice relaxation measurements. **A. Knoerdel**, S. Holmes, R. Iuliucci, C.R. Dybowski

CHED **1652.** Rovibronic quantum chemical analysis of the anion $CCNH_2^-$. **C. Stephan**, M.K. Bassett, R.C. Fortenberry

CHED **1653.** Ruthenium-based donor compounds as building blocks for proton-coupled electron transfer. **N. Odewade**, E.R. Young

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

CHED **1654.** Green graphene-in-a-blender: Facile and simple method for the production of high quality 2-dimensional materials. **B. Hatfield**, M. Puglia, C.V. Kumar

CHED **1655.** Fabrication and optical properties of aluminum nanocrescents. **C.D. Coplan**, M.M. Swartz, M. Rodriguez, S. Blair, J.S. Shumaker-Parry

CHED **1656.** Spectroscopic and computational study of chlorine dioxide/water interactions. **S. Sutton**, W.E. Cleland, N. Hammer

CHED **1657.** Improved efficiency in organic photovoltaics via luminescent/photovoltaic device coupling. **T. Morrissey**, D.A. Rider, D.L. Patrick

CHED **1658.** Supramolecular assembly of donor-acceptor energy transfer system. **E.B. Conklin**, E.R. Young

CHED **1659.** Thermal decomposition products of gas-phase acetoin. **S. Cole**, M. Ellis, J. Sowards, L.R. McCunn

CHED **1660.** Effect of pH on the reversible metachromasy of crystal violet on TiO_2. **K. Plotzke**, S. Coon

CHED **1661.** Spectroscopic and thermodynamic investigations of a mixed surfactant/polymer system at the oil-water interface. **C. Steen**, B. Schabes, G.L. Richmond

CHED **1662.** Probing local secondary structure of transmembrane alpha helices of the S21 pinholin protein using electron paramagnetic resonance spectroscopy. **R. Serafin**, D. Drew, R. McCarrick, G. Lorigan

CHED **1663.** Synthesis, NMR characterization, and kinetic studies of creatine pyroglutamate. **M. Gao**, A.S. Wallner

CHED **1664.** Molecular structure and electronic properties of anthocyanidins for use as photosensitizers. **K. Calvelo**, E.A. Jarvis

CHED **1665.** Role of low-energy (. **C. Buffo**, S. Baniya, C.R. Arumainayagam

CHED **1666.** Photodissociation dynamics of OCS at 230nm. **J. Johnstone**, W. Wei, C.J. Wallace, S.W. North

CHED **1667.** Fluorescence anisotropy decay of FMN in LOV domains from *Rhodobacter sphaeroides and Chlamydomonas reinhardtii*. **K. Marincin**, W.H. Newhart, S.K. Bailey, J. Johannsen, C.K. Johnson

CHED **1668.** Application of the Pitzer ion-interaction theory for the aqueous solution of HCl + $LaCl_3$, HCl + $PrCl_3$, HCl + $NdCl_3$, HCl + $SmCl_3$ at 25°C. **L. Roy**, R.N. Roy, D. Gregory, C. Himes

CHED **1669.** Non-resonant two-photon excitation of phototriggers. **E.R. Lorenzo**, S. Senadheera, A.L. Houk, R.S. Givens, C.G. Elles

CHED **1670.** Determination of rate constants for acetonylperoxy/hydroperoxy self reactions and cross reaction via infrared kinetic spectroscopy. **J. Cowen**, F.J. Grieman, A.O. Hui, M. Okumura, S.P. Sander

CHED **1671.** Theoretical and experimental study of CH_3SO_3H-H_2SO_4 aerosol formation. **M.D. Fellows**, H.K. Hernandez-Soto

CHED **1672.** Molecular dynamics simulations of polyisobutylene. **H. Ponce**, M.M. Fuson

CHED **1673.** Effects of sodium chloride on the behavior of methylglyoxal at the air-water interface. **G. Lindquist**, B. Gordon, N.A. Valley, S. Wren

CHED **1674.** Using evanescent-wave cavity ring-down spectroscopy and a chemical gradient to determine the free energy of adsorption of phosphotungstic acid to clean and silane-modified silica. **R.J. Korlewitz**, M.A. Everest

CHED **1675.** Temperature dependency of laser optics. **N. Almeter**, J. Orr

CHED **1676.** Covalency and rovibrational spectra of noble gas compounds. **C.M. Novak**, R.C. Fortenberry

CHED **1677.** Photodegradation of bisphenol derivatives with gold-loaded titanium oxide nanoparticles. **M. McCausland**, D. Brown

CHED **1678.** Sequential adsorption of decyl thiocyanate and octanethiol on Au(111). **D. Zoltek**, A.F. Raigoza

CHED **1679.** Raman analysis of cobalt-zirconium heterobimetallic materials. **I. Bogacz**, M. Bedford, N. Celia, A. Stone, C. Jahncke, A. Hill

CHED **1680.** Investigation of the reaction of formamide on pyrite. **N. Haddad**, H.M. Bevsek

CHED **1681.** Stabilization of hexamethylene triperoxide diamine through addition of alkyl functional groups. **C. Downing**, M. Dorko

CHED **1682.** Determining the feasibility of supercritical carbon dioxide + water for extracting organic compounds in extraterrestrial environments: A Monte Carlo simulation study. **K.J. Mei**, J.M. Stubbs

CHED **1683.** Application of the CAF to viscosity and conductivity data of solutions containing Li salt and pyrrolidinium-based ionic liquids. **C.J. Van Hoozen**, A.J. Lowry, A.M. Fleshman

CHED **1684.** Novel natural gas compressor: Interactions between water and natural gas contaminants. **D. Gallegos**, D. Brown

CHED **1685.** Using the compensated Arrhenius formalism to investigate viscosity and conductivity trends in imidazolium-based ionic liquids. **W.J. Hetcher**, A.M. Fleshman

CHED **1686.** Design and application of a novel nitrogen gas adsorption device. **S.S. Ward**, **B. Zanca**, K.E. King, A. Leenig, A. Olaitan, K.S. Molek

CHED **1687.** Effect of solid catalyst concentration in a triphase catalytic reaction. **I. Blackburn**, N. Shabestary

CHED **1688.** Pressure dependent ionic conductivity of complex lithium oxide solid electrolyte materials. **C.D. Torres**, J. Ostrander, D.C. Teeters

CHED **1689.** Evidence of Fe^+-induced decomposition of two significant greenhouse gases. **C.L. Emmerling**, A.B. Eden, W.S. Taylor

CHED **1690.** Identification of vibrational frequencies for CH_2CHI_2 and CH_3CHI using matrix-isolation spectroscopy. **M. Avina**, X. Zhang, S. Buchhorn, F.J. Grieman, S.P. Sander

CHED **1691.** MD study of the effect of alkyl aromatic content on thermophysical properties of surrogate catalytic hydrothermal conversion fuels. **M.Z. Gustafson**, B.H. Morrow, D.J. Luning Prak, S. Maskey, J.A. Harrison

CHED **1692.** Thermodynamic characterization of a novel anthracycline/DNA binding mechanism. **J. Finan**, S. Glazier

CHED **1693.** Correlation between the change in dipole moment and photosensitivity of ciprofloxacin: A better molecular predictor of photosensitivity in pharmaceutical drugs. **M. Nguyen**, A. Bills

CHED **1694.** Characterization of oxide layers on zinc selenide. **M.A. Steves**, S. Zwart, N. Hellgren, A.R. Noble

CHED **1695.** Colors in chaos: An in-depth study of chemical oscillations. **G. Misiewicz**, S. Glazier, D. Look

CHED **1696.** Unique hot carrier distributions from scattering mediated absorption. **K.R. Fernando**, J.J. Foley, N. Eldabagh

CHED **1697.** Raman spectroscopic and computational study of the electron withdrawing effects on halogen bonding. **K. Allen**, S. Nguyen, T.L. Ellington, G.S. Tschumper, D.L. Watkins, N. Hammer

Section I

Moscone Center
Hall D

Undergraduate Research Posters

Polymer Chemistry

Cosponsored by PMSE, POLY and SOCED

N. Di Fabio, *Organizer*

12:00 - 2:00

CHED **1698.** Optimizing the procedure of electrospinning an antimicrobial nitric oxide wound care patch. **D.E. Blum**, K. Malone, N. Beres

CHED **1699.** Synthesis and characterization of linear and branched valine-based poly(ester urea)s for hernia mesh repair. **L.L. Robinson**, N.Z. Dreger, M. Wade, D. Luong, M. Becker

CHED **1700.** Synthesizing amikacin containing polymers for targeted drug delivery using ring opening metathesis polymerization. **D. Urman**, R. Long, O. Ogba, D.M. Ratner, D.J. O'Leary

CHED **1701.** Dynamic Thiol–Michael chemistry for thermoresponsive rehealable and malleable networks. B. Zhang, **Z. Digby**, J. Flum, P. Chakma, J. Saul, J. Sparks, D. Konkolewicz

CHED **1702.** Preparation of sodium dodecylsulfate micelle encased polypyrrole oligomers. **G. Ahmad**, D. Moore

CHED **1703.** Effects of wound dressings on the rate of wound healing in rats. **M. Ware**, **K. Malone**

CHED **1704.** Synthesis of generation 3-bis MPA dendrimers as a platform for novel nanotherapeutic drug delivery systems. **B.V. Redmond**, J. Jackson, J. Manono, S. DiMaggio

CHED **1705.** Dispersion of pristine multi wall carbon nanotube by chain end modified poly (N-isopropyl acrylamide). **R. Francis**, N. Joy

CHED **1706.** Calixarene-core star polymers: Building blocks for micelles and drug delivery. **C.L. Turpin**, **L.L. Hepp**, P.S. Corbin

CHED **1707.** Sulfonated polyether ether ketone/expanded polyether ether ketone composite proton exchange membrane casting procedure. **E. Frampton**, J. Romeo, A. Vong, J.H. Doan, E.S. Smotkin

CHED **1708.** Electrochemical polymerization of thiophene derivatives attached to lead sulfide nanoparticle. **T. Johnson**, **M.J. Strauss**, **S.W. Steele**, J. Zemke, R.W. Kopitzke

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CHED **1709.** Investigation of doped silica aerogels for drug delivery systems. **Y.T. Paung**, M.K. Carroll, A.M. Anderson

CHED **1710.** Surface modification of ion conducting ceramic particles. **S. Veroneau**, Y. Na, R.D. Miller

CHED **1711.** Characterization of metallogels: Evaluation of thermal stability and analysis of supramolecular interactions. **N.E. Boissy**, J. Crane

CHED **1712.** Calix[4]arene-based covalent porous polymers for water purification. D. Shetty, **I. Jahovic**, A. Trabolski

CHED **1713.** Facile syntheiss of functional amphiphilic poly(valerolactone)s for drug delivery applications. **A. Morrell**, A. Yiu, J. Hao

CHED **1714.** Synthesis of functional poly(δ-valerolactone)s via post-polymerization modification. **A. Yiu**, A. Morrell, J. Hao

CHED **1715.** Lipid membrane interaction thermodynamics of cell-penetrating peptides. **A. Folska**, L.E. Prevette

CHED **1716.** Binding affinity of polycation-coated Au nanoparticles to gram positive bacterial cell walls. **H. Ganzel**, L.E. Prevette

CHED **1717.** Thermal analysis of linear high molecular weight poly-DCPD (dicyclopentadiene) and its brominated derivatives. **D. Barvaliya**, H.J. Schanz

CHED **1718.** Preparation of peptide-based biomaterials via microwave-assisted RAFT polymerization. **A.S. Magsumbol**, E.M. Giles, A. Jameson, A.F. Ennis, J.G. Schellinger

CHED **1719.** New generations of anion-responsive liquid crystals. **A. Steen**, A. Kinge, S. Cordero, L. Lam, K.A. Grabias, P. Cohn

CHED **1720.** Ionic conductivities of $LiClO_4$ polymer electrolytes for lithium-ion battery applications. **O. Vande Stouwe**, L.J. Lyons

CHED **1721.** Towards getting control: Strategies for reproducible hydrogel networks. **J. Cubuk**, M. Jani, D. Shah, **H. Zhu**, S. Qavi, R. Foudazi, S. Rajaraman, P. Cohn

CHED **1722.** Electrospinning alginate-based fibers for biomedical applications. **W.B. Weeks**, K. Penton, A. Wilson, S.K. Hamilton, G. Buschle-Diller

CHED **1723.** Diarylethene conjugated polymers: The effect of the co-monomer on photochromic and redox properties. **A. Sidari**, D.G. Patel

CHED **1724.** Phototunable azo polymers of intrinsic microporosity. **O. Chaarawi**, M. Haaf

CHED **1725.** Organic light-emitting diodes and the effects of sidechains on polymer solubility. **P. Dang**, **E. Evans**, G. Benito, A. Nguyen, C.A. Young

CHED **1726.** Differential scanning calorimetric analysis of elastomers for optimization of extended use. **A.K. Dent**, D. Lindt

CHED **1727.** Frontal polymerization of acrylate monomers. **J. Jochum**, B. McFarland

CHED **1728.** Direct arylation polymerization of benzodithiophene. **C.L. Cicha**, T.M. Pappenfus

CHED **1729.** GPC Analysis of styrene polymerization using various initiators for undergraduate polymer laboratory. **G. Pearson**, K. Allen

CHED **1730.** Electropolymerization and characterization of polyaniline-TiO_2 nanocomposites for corrosion protection. **E. Taylor**, A.O. Sezer

CHED **1731.** Conjugate number effects on nanoparticle activity and stimuli response. **J. Jackson**, B.V. Redmond, J.N. Shropshire, J.M. Manono, S.C. Dimaggio

CHED **1732.** Using multi-step synthesis for the production of hydrogels with adhesive properties. **M. Alcantar**, J.M. Deardorff, C.H. Lisse

CHED **1733.** Synthesis of synthetic mimics enriched tryptophan copolymers for the use in antimicrobial studies. **J. Ewing**, S.G. Mankoci, A. Joy

CHED **1734.** Analysis of solvent storage properties of polyurea-shell microcapsules containing a free-radical initiator core. **T. Halligan,** B. McFarland

CHED **1735.** Synthesis of 1st and 2nd generation PAMAM (polyamidoamine) dendrimers. **P. McClimon**, D.J. Oostendorp

CHED **1736.** Synthesis of kanamycin ROMP polymers for site-specific drug delivery. **R. Long**, D. Urman, O. Ogba, D.M. Ratner, D.J. O'Leary

CHED **1737.** Nitrogen containing graphitic-like materials. **J. Brophy**, J.O. Hoberg, B.A. Parkinson

CHED **1738.** Synthesis of stimuli-response nanomaterials as potential drug-delivery agents. **J.N. Shropshire**, K. Watson, B.V. Redmond, J. Jackson, J. Manono, S. DiMaggio

CHED **1739.** Study of the active form of the polymerization catalyst formed between Tp*Rh(cod) and phenylacetylene using MALDI-TOF-MS. **W.J. Buck**, **J.D. Freeman**, R.M. Tarkka

CHED **1740.** Characterization and optimization of expanding foams. **T. Naudet**, D. Cuomo, D.E. Riegner

CHED **1741.** Castor oil as a renewable alternative to poly(ethylene oxide) in isosorbide-derived thermoset polymers. **J. Swartz**, P. Wilbon, J. Brutman, M.A. Hillmyer, J.E. Wissinger

CHED **1742.** Controlled polymerization of D,L-lactide with a titanium(IV) tartrate. **B. Benson**, B.M. Chamberlain

CHED **1743.** Withdrawn.

CHED **1744.** Synthesis and characterization of polyaniline-MnO_2 nanocomposite for supercapacitors. **K. Hager**, A.O. Sezer

CHED **1745.** $NdCl_3$ 3TEP-TIBA catalyst system for coordination polymerization of diene and vinyl monomers. **A. Yang**, R.N. Kularatne, M.C. Stefan

CHED **1746.** Characterizing oligo (ethylene oxide) oxanorbornyl homopolymers and diblock copolymers for solid electrolyte supports. **R.A. Zhuravlev**, D.A. Waldow

CHED **1747.** Removal of organic micropollutants in water with a microporous polymer as a platform for an undergraduate teaching lab. **E. Bravo**, M. Haaf, A. Alsbaiee, M. Klemes, W.R. Dichtel

CHED **1748.** Nanostructured lithography through self assembly of diblock copolymers. **L.R. Steiner**, A. Christy, J.D. Harris, D. Estrada

CHED **1749.** Withdrawn.

CHED **1750.** Toward photochromic nanohybrids based on upconverting nanoparticle: Nanocargos for drug delivery. **S. Zaid**, C. Coudret

CHED **1751.** Biomedical applications of thiol-acrylate polymerization. **J.Z. Gombeda**, L.A. Garber, J.A. Pojman, D. Hayes

CHED **1752.** Design of supercapacitor separators based on polymeric-ceramic bio/composites: Enhancing performance for applications in biomedical implantable devices. E.O. Ortiz Quiles, **C.O. Alvarez- Sanchez**, J. Lasalde-Ramírez, R. Masso-Ferret, E. Nicolau

CHED **1753.** Improving properties of poly-valerolactone through aryl ring stacking. **P. Sitarik**, K. Allen

CHED **1754.** Synthesis of nanocrystal polymer ligands for dispersant-free LSCs. **F. Son**, D.A. Rider, A. Morren, D.L. Patrick

Hollyweird Chemistry

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The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit

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MONDAY EVENING

Section A

San Francisco Marriott Marquis
Salons 1/2

Innovating Materials for the Next Generation: Bringing Practical Applications into the Chemistry Classroom

Cosponsored by PMSE, POLY and RUBB

Financially supported by IPEC

S. C. Rukes, *Organizer, Presiding*

5:00 Introductory Remarks.

5:05 CHED **1755.** Materials, materials: They are everywhere. **E.J. Escudero**, **S.C. Rukes**

5:25 CHED **1756.** Cars: A rolling evolution of material choices. **A. Nydam**, **S.C. Rukes**

6:05 Intermission.

6:10 CHED **1757.** Evolution of aircraft materials: Why are we building plastic airplanes? **A. Nydam**, **S.C. Rukes**

6:50 CHED **1758.** Polymers, polymers everywhere. **D. Moore**

7:30 Intermission.

7:35 CHED **1759.** Chemistry connections: Inspiring students with innovation. **K. Anderson**, M. Enright

8:15 CHED **1760.** Composites and conductive materials: Making everyday materials do more. **S.C. Rukes**

8:30 CHED **1761.** Nanotechnology for drug delivery. **S.C. Rukes**

8:45 Concluding Remarks.

Section B

Moscone Center
Hall D

Successful Student Chapters

Cosponsored by SOCED

N. Di Fabio, *Organizer*

8:00 - 10:00

CHED **1762.** Mississippi College ACS Student Chapter. **A. Smyly**, **B. Nash**, **S.G. Travis**, T.D. Selby

CHED **1763.** Chemistry within the community: Successful student chapter at Eastern University, PA. **A. Crawford**, **K. Martinez**, J. Bundens

CHED **1764.** Observing the effect of STEM outreach for grade 5-8 students through the Bridgewater State University chemistry club. **K. Dooley**, **P. Kurriss**, E.J. Brush

CHED **1765.** Erskine College ACS student chapter: Outreach constantly, not periodically. **K. Squiggins**, A. Houston, T. Hayden, J.E. Boyd

CHED **1766.** Universidad del Sagrado Corazon ACS Student Chapter: A new engine for chemistry in our society. **J.M. Rosado**, I.J. Ovalle, B.M. De Llovio

CHED **1767.** Scientific community involvement. **B. Esterlen**, B.J. Bellott

CHED **1768.** Missouri Western State University Alchemist Club: Transmuting students into scientists. **J. Moore**, **J. Wagner**, M. Svay, N. Chapman, D. Stasko

CHED **1769.** Building a successful ACS student affiliate through community outreach, community service and professional development. S. Cunninham, D. West, N. Elmore, H. Hsieh, R. Ali, T. Nielsen, R. McFarland, **R.V. Valcarce**, P.J. Iles, L. Giddings, N.R. Bastian, W. Sanders, S. Richards, M. Alvarez, R. Holcomb

CHED **1770.** Increasing interest in chemistry. **J. Kuang-Nguyen**, R. Hutchison, J.A. Darsey, D. Soni, O. Cossio

CHED **1771.** Successful ACS student chapter at Wilkes University: Community outreach events that apply green chemistry principles and science education. **J. Colvin**, R. Hohol

CHED **1772.** Morehead State University. **B. Knicely**, M.T. Blankenbuehler

CHED **1773.** Saint Vincent College Chemistry Club. **J. Centore**, D. Fish, B. Tomiczek, G. Ngo, D. Carone

CHED **1774.** Keep calm and make bonds: Chemistry at Xavier University of Lousiaina. **V.C. Miles**, T. McClelland, **S. Bertrand**, **D.D. Daley**, **J. Adkins**, **I. Gill**, **M. Ndukwe**, **B.V. Redmond**, M.R. Adams, C.M. Lawrence

CHED **1775.** ACS-San Germán Chapter: Sustainable growth. **A. Acosta**, **E. Franceschini-Silva**, **R. Flores-Morales**, **N. Irizarry,** M. Jusino, M. Martinez-Mercado, I. Otero, C. Perez-Rodriguez, P. Silvestry, S. Vargas-Padilla, E. Velez, N. Caraballo, A.M. Gonzalez

CHED **1776.** ACS UPR–RP Student Chapter: Inspiring tomorrow's society through chemistry. **R. Colon Morillo**, A. Gonzalez Lopez, F. Serrano Martinez, N.I. Alvarez Colon, C. Aponte Ortiz, M. Rivera Cora, K.M. Collazo Maldonado, J. Cosme Silva, E. Pagan Colon, D. Rosario Berrios, L.S. Martir Ramirez, L.A. Nieves Santiago, T.M. Dominguez Gonzalez, E. Albino Rivera

CHED **1777.** SIUE Chemistry Club: Spreading chemistry knowledge on campus and in the community. **E. Baldwin**, B. Florea, H. Lupton, K. Link, E. Ross, M.W. Jones

CHED **1778.** Angelo State University Green Chemistry Student Chapter. **A.F. Sullivan**, B.R. Holle, D. Herrick, K.A. Boudreaux, E. Osborne

CHED **1779.** Saint Francis University Chemistry Club: Don't worry about it dad. R. Krupa, H. Schorr, W. Shee, **E.P. Zovinka**

CHED **1780.** Santa Monica College Chemistry Club: A growing student chapter. **S. Purucker**, **C. Vaughan**, **M. Martinez**, T. Pecorelli

CHED **1781.** Otterbein Student Chapter. **E. Isaac**, R. Grote, J.M. Esson

CHED **1782.** South Dakota School of Mines and Technology: A successful student chapter of the American Chemical Society based on outreach and education promoting an appreciation of chemistry. **T. Johnson**, **K. Giorgio**, J. Meyer, T. Ryther, S. Jenkins, H. Leppert, M. Acevedo

CHED **1783.** Eastern Oregon University ACS Student Member Chapter: Promoting community outreach and professional networking. **D. Spikerman**, **B. Mandella**, **C.J. Burghard**, **A. Courtois**, A.G. Cavinato

CHED **1784.** DeSales University's ACS student chapter activities during the fall 2015 and spring 2016. F.C. Mayville, **E.N. Sauschuck**, **A.M. Myers**

CHED **1785.** Chemistry in the Heidelberg University community. **A.F. Bauer**, C. Chandler, K. Scrudders, D.E. Blum, M.N. Hogle, E.N. Riffle, N. Beres

CHED **1786.** ACS Inter Ponce Student Chapter Forensic Chemistry Division. **R.M. Perez-Ortiz**, M.A. Reyes Caraballo, Y. Santos-Vazquez, G.M. Santiago Rivera, J.I. Ramirez Domenech, E. Ferrer Torres

CHED **1787.** Pasadena City College Chemistry Club. **L. Lupercio**, **L. Ramirez**, **D. Cagan**, **V.I. Jaramillo**

CHED **1788.** Chemistry, the Flint Water Crisis, and you. **C. Wilhelm**, **A. Maxwell**, **D. Corey**, **N. Alawwa**, **M. Alsarraj**, **W. Yahr**, **T. Sanson**, M.R. Wilhelm, J.L. Tischler, S.S. Grathoff

CHED **1789.** University of Minnesota, Morris ACS Chemistry Club: Chemistry beyond the classroom. **H. Goemann**, D. Schultz

CHED **1790.** Loras College American Chemical Society affiliated Chemistry Club. C. O'Bryan, B. Al-bazboz, **B. Anderson**

CHED **1791.** Withdrawn.

CHED **1792.** Mission of the College of Mount Saint Vincent science club. **B. Hoyland**, **W. Lang**, P. Nunez, P.K. Kerrigan

CHED **1793.** Canisius College Student Chapter of the American Chemical Society. **W.B. Swanson**, L.T. Evans, C.B. Tumiel, T.M. Tumiel, P.M. Sheridan

CHED **1794.** Leading a successful ACS student chapter. **D. Lewis**, **L. Louis**, A.J. Sanders

CHED **1795.** TCU Chemistry Club: Effective organization and communication methods for outreach. **S. Price**, **A.T. Vu**, **H. Villegas**, **E.V. Akhimien**, **M. Barnett**, **K. Upton**, **B. Niebuhr**, **A. Hassan**, **C.N. Simmons**, **I. Al Farra**, **N. Schmitt**, B.G. Janesko, K.N. Green, J. Fry

CHED **1796.** Chemistry is central at the University of Central Oklahoma: Successful student chemistry club chapter activities. A. Arnold, C.D. Fleming, K. Kordsiemon, G.S. Rodriguez, D.R. Rundle, **C.B. Frech**

CHED **1797.** Mythbusters: The age old question, fact or fiction? **T.J. Orr**, **S.A. Armstrong**, J.D. Hall, J.L. Sims, J.T. Jatko, R.J. Baltz, B.A. Kelley, Q. Saunyama, G.D. White, K. Ding

CHED **1798.** University of Tennessee at Martin student member chapter. **T. Rinehart**, W.L. Kuenzinger, M.E. Short, B. Ide, S. Oliva, A.H. Shelton

CHED **1799.** Growing the student affiliate chapter at Ferris State University. **T. Stothers**, **J. Goyola**, M.A. Thomson

CHED **1800.** Development of an active and engaged chemistry club. **S. Pribil**, K. Sorauf

CHED **1801.** Aquinas Chemistry Society. C.R. Jensen, **A. Wagner**, **J. McAfee**, B. Arnson, A. Brock, E.A. Jensen

CHED **1802.** Emergent Point: Becoming chemistry citizens. **A. Almodovar Ortiz**, Y. Cruz Reyes, J.I. Ramirez Domenech, E. Ferrer Torres

CHED **1803.** Sacred Heart University Student Affiliates are salt bridging chemistry into the community coast to coast. **S. Aanonsen**, **S. Baer**, **C. Domville**, **C. Inferrera**, **F. Divisconti**, **R. Russo**, **S. Zupetz**, **M. Filja**, H. Jia, C. Rose, B. Kalach, L. Farber

CHED **1804.** ACS Student Chapter at The University of Texas at Tyler. **P. Hightower**, R. Williams, L. Johnson, L.E. Boyd

CHED **1805.** Best of both worlds: Adapting Detroit Mercy Chemistry Club activities to incorporate urban and suburban surroundings. **M.J. Mio**, R. Beltman, S.M. Fudalla, D.N. Maxwell, G. Nguyen, J. Pothoof, K.M. Suiter, R. Zouabi, K.R. Evans

CHED **1806.** Igniting change: Gordon College's ACS chapter's influence on campus and the community. **I. Ngo**, V. Curfman, L.T. Walsh, K. Elliott, E. Percival, I.J. Levy

CHED **1807.** Fostering a successful ACS chapter at a private liberal arts institution. **A. Narro**, D. Chavez, D. Ivan, J. Belmares, A. Roth-Rodriguez, M. Kopecki Fjetland

CHED **1808.** Chemistry Club: Coming together to synthesize a brighter future. C. ACS Student Chapter, **A.P. Zurmuhle**, N. Eddy, J. Tran, P. Rodas, S. Jinata, G. Singh, **B.F. Gherman**, C.J. Kellen-Yuen

CHED **1809.** Student Members of the American Chemical Society: Hofstra Chapter 2016-2017. **S. Kim**, A. Gaglio, M. Chambers, M. Kaur, A. Sica, A. Xiang, M. McNamara

CHED **1810.** Small liberal arts college approach. **J. Tobin**, H. Fasiang, A. Horowitz

CHED **1811.** Molloy Chemical Society at Saint Joseph's University. **R. Kontos**, **C. Stow**, **M. Graziani**, A. Sargent

CHED **1812.** ChEmory: Emory University's undergraduate chapter of the American Chemical Society. **S. Gupta**, J. Fu, D. Salgueiro, K. Woolard, A. Kim, D.R. Mulford

CHED **1813.** Promotion of a chemistry major identity through the Student Chemists Association at The College of New Jersey. **K.M. Fomchenko**, **T.M. Townsend**, **M. Casale**, A.R. O'Connor, B.C. Chan

CHED **1814.** Student Affiliates of the American Chemical Society: Washington & Jefferson College 2016. J.D. Goltz, **A.M. Krol**, T. Yeung, J. Hosfelt, D.A. Polvani

CHED **1815.** Student members of the American Chemical Society: University of Arizona Chapter. **S. Avetian**, J. Lopez, J.R. Pollard

CHED **1816.** Angelo State University ACS Student Chapter. **D. Herrick**, A.F. Sullivan, E. Osborne, K.A. Boudreaux

CHED **1817.** Barry University Chemistry Club: Sharing our passion for chemistry. **E. Paulus**, D. Cordero, N. Maxi, R. Gutierrez, T.D. Hamilton, G.H. Fisher

CHED **1818.** Methods to improve university student engagement and contribution to scientific enrichment. **N. Diaz**, H.R. Aguilar

CHED **1819.** Chemistry and camaraderie: Student activities at the University of New England. **M. Wright**, **J. Woolf**, **B. Rivard**, A.E. Keirstead

CHED **1820.** Activities of the Monmouth University Chemistry Club. **K. Muratore**, B. Macalush, O. Adetunji, A. Scorzelli, G.A. Moehring, D. Szwajkajzer

CHED **1821.** University of Northern Iowa ACS Student Chapter: Creating successful chemists. **A. Wold**, E. Dutton, J. Nederhoff, W.W. Andersen, M. Flesch, K. Plotzke, J. Prybil

CHED **1822.** University of Utah ACS Student Chapter. **A.M. DeGrauw**, T. Xu, R. Reynolds, S. Lee, M. Pham, W.E. Scholl, A. Loret, H.L. Sebahar, T. Richmond

CHED **1823.** University of Tampa American Chemical Society Chapter's outreach in the greater Tampa Bay area. W. Smith, **N. Zembol**, L. Henchey, J.A. Struss

CHED **1824.** Solving the mystery of chemistry: Illinois Valley Community College Chemistry Club. **K. Murphy**, **T. Perry**, **J. Meyer**, **S. Nelson**, **A. Ochuba**, **G. Braboy**, M.E. Johll, P.K. Yong

CHED **1825.** Strategic anabolic reaction: Incorporation of a Division of Biotechnology to the ACS student chapter from the Interamerican University of PR Ponce Campus. L. Rivera Vazquez, **J. Costas Feliciano**, M. Barriera Diaz, J.I. Ramirez Domenech, E. Ferrer Torres

CHED **1826.** Coloring the minds of our youth through chemistry. **K. Weeber**, N. Lygeris

CHED **1827.** Suffolk University engaged with chemistry 2016-2017. **K. Jenkins**, K. Vu, A. Biyari, J. Bautista, N.M. Reed

CHED **1828.** Chemistry marathon! **J.K. Vale**, L. Santos

CHED **1829.** Green legacy: An optimal alternative for the UPR-Aguadilla. **K. Negron-Teron**, **W. Lopez-Perez**, B.J. Ramos-Santana, C.R. Ruiz-Martinez

CHED **1830.** Putting the fun in funding: Finding new ways to fund the Detroit Mercy Chemistry Club. **M.J. Mio**, R. Beltman, S.M. Fudalla, D.N. Maxwell, G. Nguyen, J. Pothoof, K.M. Suiter, R. Zouabi, K.R. Evans

CHED **1831.** Starting the year off with several bangs: The ACS Student Chapter at Sacramento City College. **A. Thomas**, S. Cook, I. Qureshi, G. Cruz-Velasquez, N. Le, V. Alino, W.J. Miller

CHED **1832.** Solving mysteries through chemistry. **T. Williams, A. Hudson, D. Whitman,** C.K. Saner

CHED **1833.** Expansion of the sphere of influence: KU Chemistry Club member recruitment and retention. **R. Latimer**, E. Lorenzo, P.R. Hanson, R.S. Black

CHED **1834.** Successful student chapter: University of New Mexico student chapter of the American Chemical Society. **A. Rauch**, **J. Platero**, **K. Thompson**, **J. Meyer-Hagen**, **J. Terr**, L.J. Whalen

CHED **1835.** Northeastern University Student Affiliates of the American Chemical Society: Building connections and foundations within our communities. **J. Compton**, B. Laramee, C. Gallin, T. DeLano, **D. Dang**

CHED **1836.** Building professionals through their involvement with the FIU BBC-Science Club. **M. Michel**, S.N. Ike, J. Glenny, C. Cazimir, K. Pierrelouis, D. Read, V. Perez, M. Delgado, M. Exposito

CHED **1837.** Centenary College of Louisiana: A tradition continued. **V. Robert**, H. Deshautelle, G. Doucet, M. Abo-Zahrah, T.M. Ticich

CHED **1838.** SMACS @ FSU. **A. Lette**, **B.M. Day**, B.N. Norris

CHED **1839.** Park University CHEM club success 2016-2017. **J. Pham**, **G.S. Stelmacovich**, **A.N. McMullen**, **M.M. Klein**, **D.K. Howell**, **G.D. Claycomb**

CHED **1840.** Creating bonds within the UCSD American Chemical Society - Student Affiliates. **D. Nguyen**, T.J. Bussey, S. Brydges

CHED **1841.** American Chemical Society Student Chapter at the University of St. Thomas, Houston, TX. **P. Zaibaq**, A.V. Hernandez, N.B. Nguyen, T.J. Pham, M. Guirette, K. Vazquez, C.A. Young, J. Hollingsworth

CHED **1842.** Colorado State University Chemistry Club: Collaborate, network, and connect. **R. Schiffhauer**, J. Brookhart, A. Detmer, N. Knostman, L. Monterrosa Zavaleta, L. Paricio, M. Plonski, A. Rauker, I.M. Sitarik, B.P. Reynolds

CHED **1843.** Achievements of KSU SAACS in fall 2016 for students in chemistry-related fields and local educational institutions. **P. Jean**, **A. Calderon**

CHED **1844.** Using chemistry as a tool to stimulate interest, engage minds, encourage involvement and motivate to achieve. **A. Almaguer**, **C. Garcia**, M. Zamora, T.M. Rodriguez, U. Swamy

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CHED **1845.** Carroll University Chemistry Club. **N.P. Biewer**, C. Garcia, K. McCarthy, L. Glodowski, C. Kraska, R.M. Kutzner, V.M. Wartenweiler, K.E. Molter

CHED **1846.** Efforts of a chapter to preserve its Outstanding award: The ACS Student Chapter of the University of Puerto Rico at Cayey. **W.M. Lopez**, M. Leon, E. Rivera Tirado

CHED **1847.** Western Washington University Student Chapter of the American Chemical Society. **C. Crickmore**, R. Blazevic, **S.R. Emory**, E. Raymond

CHED **1848.** Santa Clara University Student Member Chapter: Creating a successful balance of events to promote student involvement in the chemistry community. **C. Dubois**, J. Yin, **L.S. Brunauer**

CHED **1849.** Success through serving and sharing is instrumental: A Waynesburg experience. **K. Wilson**, B. Bosley, A. Narehood, K. Houser, J. Gearhart, E.A. Baldauff

CHED **1850.** Science is universal. **C. LeBlanc**, M. Yurkevicius, C. Murphy, S.K. O'Shea

CHED **1851.** Gruen Chemistry Society: Student affiliate activities at Olivet College. **M.C. Carr**, **K.J. Nault**, **E.R. Cole**, **J.L. Elliston**, S.M. Lewis

CHED **1852.** Truman State University Student Affiliate Chapter. **S. DeBie**, **L. Chapman**, T. Humphry

CHED **1853.** Chronicles of the jurassic outreach expedition in south Texas. **M. Ochoa**, A. Chrysler-Martinez, A. Hut, K. Moreno, **L. Avila**

CHED **1854.** Dynamic activities of the ACS student chapter at Inter American University of Puerto Rico - Metropolitan Campus. K.A. Parga Rivera, **K.A. Lopez-Perez**

CHED **1855.** Broadening the undergraduate impact of Nittany Chemical Society. **C. Poirier**, G. Leone

CHED **1856.** Activities for the Henderson State University student affiliate chapter. **W. Garrett**, **J. Stephens**, D. Bateman, B.A. Rowland

CHED **1857.** Student Affiliates of the American Chemical Society - South Dakota State University. **F. Poppinga**, **A. Kub**, **L. Dirks**, **J. Soukup**, **M. Radtke**

CHED **1858.** Celebrating NCW 2016 at University of Puerto Rico Humacao. **L. Flores**, A. Figueroa, J. Ramos, K. Orta, O. Rivera, J. Suarez

CHED **1859.** Ouachita Baptist University Student Chapter: Sharing chemistry. **J.C. Bradshaw**, A. Cole

CHED **1860.** Warriors Chemistry Club at Stanislaus State: Inspiring the next generation through chemistry awareness. **J. Vivar**, **K. Chan**, J.Y. Lo, S.K. Mendez, J. Godinez, K. Soares, E.A. Alemán

CHED **1861.** Lock Haven University of Pennsylvania Chemistry Club. **S. Shreiber**, T. Adams, S. Sujansky, K. Range

CHED **1862.** SMSU Chemistry Club: Inspiring future chemists one hydrogen balloon at a time. **R.M. Sears**, **M.M. Bruns**, **V.J. Henry**, N.J. Beyer

CHED **1863.** Chain reaction: Impacting the community through chemistry. **G.E. Alvarez**, **T. Massas Le'Cleres**, **I. Rios Cruz**, **R.M. Zamora**, **A. Rivera**, **O. Alvarez**, **M. Rodriguez**, **A. Cruz**, **P. Velez Vega**, **P. Maldonado**, **P. Goyco**, **L. Perez**, **C. Beauchamp Perez**, **N.E. Crespo Rosado**, **D. Cordero DaSilva**, **A. Altiery**, **N. Tristani**, J. Torres Candelaria

CHED **1864.** American Chemical society student chapter at Peninsula College. **B. Weintraub**

CHED **1865.** Professional development through industrial speakers. **C.M. Schreidah**, **J. Fife**, **E. Kenney**, **J. Culp**, **M. Klingberg**, **S. Cassidy**, **A. Prokay**, **G. LaFleur**, E.P. Kippenhan

CHED **1866.** American Chemical Society Student Chapter of Idaho State University. P. Ropski, S. Spradlin, B. Poulter, E.A. Morley, **W.C. Spence**, J.J. Pak, C.M. Evilia

CHED **1867.** Kappa Epsilon Mu (K.E.M) Club at Texas Woman's University: Reaching the community through chemistry. **K. Slavens**, D.B. Hernandez, T. Nguyen, S. Scott, K. Reyes, N. Mirsaleh-Kohan

CHED **1868.** Creating a triple bond: Linking PLU students with professional development, community outreach, and green chemistry. K. Cameron, O. Egejuru, C. Flanery, J. Wong, **A.M. Munro**

CHED **1869.** ACS Student Chapter at the University of Central Florida. R. Sapia, S.M. Kuebler, **J. Lear**, P. Velez, M. Tedlie, G. Versfeld, P. Vazquez

CHED **1870.** Illinois State University ACS Student Chapter year in review 2015-2016. **A. Bruno**, W.T. Darrow, A. Mandl, A.N. Latham, E. Jugovic, Z.E. Lawton, S. Huffman

CHED **1871.** For the students, by the students: Actively working to develop resources for CMU chemistry undergrads. **S. Bedford**, **J. Groenevelt**, **J. Callus**

CHED **1872.** Club activities and community outreach by ACS student chapter of Midland College. **Z. Hunter**, M. Ennis, K. Marrufo, A. Jones, S. Esan, J. Espinoza, D. Gable, J. Anderson, P. Nandakumar

CHED **1873.** Wayne State University American Chemical Society Student Affiliates. **Y.K. Elghoul**, A.R. Breckenridge, A. Dao, J.L. Stockdill

CHED **1874.** ACS UMET chapter: Engaging undergraduate students, pre-colleges, and kids for science through chemistry activities. **A.C. Aponte**, **J.G. Medina-Feliciano**, B. Hopgood, J. Morales, O.M. Primera-Pedrozo, M. Falero-Gil

CHED **1875.** When things go wrong: Navigating the realm of insurance and liability in student chapters. **S. Taylor**, **N. Higdon**, L. Laverman

CHED **1876.** Inception of an ACS Student Chapter at San Diego Miramar College. **G.L. Smith**, L. Yang, M. Troester, M.K. Antisdel

CHED **1877.** Southeastern Oklahoma State University ACS Student Members: 50 Years of chemistry from the savage storm. **E.P. Landers**, **L. Chandler**, **K.L. Gaskill**, **P.S. Whitehead**, M.D. Madewell, S.A. Eaves, **N.L. Paiva**

CHED **1878.** Delta State University ACS gives back: National Chemistry Week. **A. Camarillo**, A. Griffin, K. Penton, W.B. Weeks, S.K. Hamilton

CHED **1879.** ACS-UPRB Walking towards new directions by improving education in green chemistry. V.M. Blasky-López, **J.C. Estarellas San Miguel**, **N.I. Estarellas-San Miguel**, **R. Gracia-Colón**, **A. Muñiz-Santiago**, **B. Padilla-Maldonado**, **K. Rodríguez-Robles**, J. Oyola Cintron, L.I. Santiago-Pérez

CHED **1880.** UCA ACS: Serving as chemistry ambassadors in Central Arkansas. R. Mayo, J. DeYoung, **S. Margis**, R. Senn, **S. Turner**, G.R. Naumeic, K.L. Steelman, F.M. Yarberry

CHED **1881.** Cooking up a love for chemistry through culinary, mentoring, and community outreach events. **J. Ulrich**, **L. Posada**, **K. Bolduc**, **B.L. Gay**, **J. Partridge**, A. Huisman

CHED **1882.** GGC game changing: Georgia Gwinnett College chemistry outreach. **D. Breaud**, **K. Coscia**, **N. Davis**, **W. Jones**, **A. Ko**, **J. Massey**, **J. Moon**, R.K. Kalman, G.E. Rudd

CHED **1883.** Student Chapter of the American Chemical Society at Minot State University. **S. Park**, H. Lee, J. Torgunrud, S. Sundhagen, B. Hatfield, E.Y. Mojica, T. Dostert, T.A. Skinner

CHED **1884.** ACS UPR-Aguadilla: The challenge of innovation from the legacy to the future. **R. Pitre-Yulfo**, **M.S. Arocho-Caban**, B.J. Ramos-Santana, C.R. Ruiz-Martinez

CHED **1885.** Florida Southern College ACS student chapter growth 2016-2017. **I. Mauzy**, S.F. Wilson, K. Martinet, A. Branch, M. Hewett, K. Alexander, J.F. Eubank

CHED **1886.** Green island promoting green chemistry. **C.G. Cortes Bula**, C. Torres Martinez, A. Almodovar Ortiz, J.I. Ramirez Domenech, E. Ferrer Torres

CHED **1887.** UTPB Chemistry Club: Promoting chemistry in West Texas. **C.B. Taylor**, R. Maharaj, J. McDonald, D. Vinson

CHED **1888.** Demos in the den: Visual demonstration of chemistry in an auditorium. **M. Sautter**, **D. McKinzey**, L. Gao

CHED **1889.** Solving mysteries through chemistry. **A. Bajaj**, M.J. D'Souza

Section C

Moscone Center
Hall D

Sci-Mix

I. J. Levy, T. A. Miller, C. M. Muzzi, *Organizers*

8:00 - 10:00

128, 136, 138, 142, 149, 152, 155, 159-160, 168, 172, 178, 187, 189, 192-193, 333, 344, 369, 393, 464, 468, 474, 509, 580, 589-590, 592, 644, 669, 721-722, 754, 767, 774, 778, 790, 793, 812, 814, 826, 835, 838, 889, 892, 896, 913, 919, 961, 965, 967, 997, 1003, 1037, 1055, 1113, 1121, 1150, 1175, 1219, 1238, 1241, 1259, 1305-1306, 1331, 1333, 1340, 1385, 1387, 1422, 1429, 1433-1434, 1475, 1510-1511, 1526, 1545, 1549, 1589, 1592, 1607, 1620, 1631, 1642, 1648, 1654, 1689, 1695, 1699, 1721, 1725, 1746, 1748, 1751-1752. See previous listings.

TUESDAY MORNING

Section A

San Francisco Marriott Marquis
Salons 1/2

George C. Pimentel Award in Chemical Education: Symposium to honor Thomas A. Holme

S. Bretz, *Organizer*

M. Cooper, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **1890.** Silent students in the active learning chemistry classroom. **J.S. Hutchinson**, C. Owens, A. Munson, L. Tran Lu, K. Kincaid

8:55 CHED **1891.** Chemical education: To infinity and beyond. **M.D. Koppang**

9:15 CHED **1892.** Identity, intersectionality, and the culture of science. **M.G. Grunert Kowalske**

9:35 Intermission.

9:45 CHED **1893.** Measuring chemical representations use among organic chemistry students to understand how they interpret different aspects of molecular structures. **J. Baluyut**, **J. Polifka**, T. Holme

10:05 CHED **1894.** Utilizing the Anchoring Concepts Content Map to track chemistry students' concept development and retention rates in general chemistry and organic chemistry. **C.J. Luxford**

10:25 CHED **1895.** Comparison of representation use in biochemistry textbooks and associated assessment questions. **K.J. Linenberger Cortes**

10:45 Intermission.

10:55 CHED **1896.** Aligning assessments: Advancing the capacity for criterion-referenced chemistry assessments. **J.J. Reed**

11:15 CHED **1897.** Chemistry assessment in the digital age. **L. Lockwood**

11:35 CHED **1898.** No Holme is an island: Systems thinking in chemistry education. **P.G. Mahaffy**

Section B

San Francisco Marriott Marquis
Salons 3/4

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Saundra Y. McGuire

Cosponsored by CMA and WCC

I. M. Warner, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 CHED **1899.** LSU LA-STEM research scholars program: Reflections on program origin and early interactions with Professor Saundra McGuire. **I.M. Warner**, M.B. Crawford, S.E. McGuire, Z.S. Wilson-Kennedy, G. Thomas

9:05 CHED **1900.** How to mentor students, support achievement, and lose weight: The remarkable mentoring of Saundra Y. McGuire. **M.H. Towns**

9:30 CHED **1901.** Designing metacognition-based learning strategies to aid in the recruitment, retention, and graduation rates of STEM students with specialized learning accommodations. **A. Kelley**

9:55 Intermission.

10:10 CHED **1902.** Chronic underrepresentation in STEM? Fix our institutions, not our students. **J.T. Matsui**

10:35 CHED **1903. Award Address** (ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences sponsored by The Camille & Henry Dreyfus Foundation, Inc.). Metacognition: The key ingredient for academic success for underrepresented (and all) students! **S.E. McGuire**

11:20 Concluding Remarks.

Section C

San Francisco Marriott Marquis

Salon 5

GSSPC: Water Sustainability

Chemists in Pursuit of Clean Water

Cosponsored by CEI and PRES

Financially supported by Georgetown University Department of Chemistry, Graduate Education Advisory Board

I. Brekalo, J. P. England, Z. S. Sakhaei, *Organizers*

A. Adcock, Z. De los Santos, S. E. Ingram, *Organizers*, *Presiding*

J. Nelson, *Presiding*

8:45 Introductory Remarks.

8:50 CHED **1904.** Chemical contaminants in drinking water - from risk to rule. **C. Sham**

9:20 CHED **1905.** Aquatic photochemistry: Pollutants, products, and policy. **K.P. McNeill**

9:50 CHED **1906.** Safe and sustainable drinking water: How can we do it? **S.D. Richardson**

10:20 Intermission.

10:35 CHED **1907.** Supramolecular receptors for anions: The commercialization pathway of a nitrate-sensing molecule towards pollution prevention in precision agriculture. **D.W. Johnson**

11:05 CHED **1908.** Technologies for enabling water reuse. **J. Wilbur**

11:35 Concluding Remarks.

Section D

San Francisco Marriott Marquis

Salon 6

Advances in e-Learning & Online Chemical Education

D. A. Canelas, L. A. Morsch, *Organizers*

P. Sorensen, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1909.** Lessons learned in 16 years of teaching chemistry online with a hands on laboratory component. **R.R. Klepper**

8:55 CHED **1910.** CCCE OLCCs. **R.E. Belford**, J.L. Muzyka

9:15 CHED **1911.** Refining online chemistry strategies. **J.E. Alexander**, **J.J. Wenz**

9:35 Intermission.

9:55 CHED **1912.** Using traditional and 3D printed physical models in an online introductory chemistry course. **J.D. Mendez**

10:15 CHED **1913.** Develop-your-own dynamic and engaging YouTube channel as an Open Educational Resource (OER) supplementing general and organic chemistry courses. **D. Jackson**

10:35 CHED **1914.** From chemists know to shredded science: Using accessible online outreach videos to ignite interest in and aid understanding of chemical concepts. **G. Grazioli**

10:55 Concluding Remarks.

Section E

San Francisco Marriott Marquis

Nob Hill A

Advances in Teaching Organic Chemistry

S. F. Hornbuckle, *Organizer, Presiding*

8:30 CHED **1915.** Using YouTube to promote student self-reflection in organic chemistry. **D. Konkolewicz**

8:50 CHED **1916.** Working smarter, not harder: Teaching organic chemistry. **S. Tong**, R.M. Kissling

9:10 CHED **1917.** Reducing extraneous cognitive load in undergraduate organic chemistry: Redistribution, not reduction. **C. Filloux**

9:30 Intermission.

9:45 CHED **1918.** Integrating biological applications into the organic chemistry laboratory using affordable instrumentation. **E. Nam**, M.P. Hill

10:05 CHED **1919.** Design and evaluation of a mobile learning paradigm aimed at improving organic chemistry laboratory instruction at undergraduate level. H. Weizman, **S. Wang**

10:25 CHED **1920.** Investigating student misconceptions in understanding acid-base reactions in undergraduate organic chemistry courses using various formative and summative assessment tools. **M. Chatterjee**, L. Katz, H. Shaaban, R. Ruvinsky

10:45 Intermission.

11:00 CHED **1921.** Undergraduate teaching assistants as part of the teaching-service model in large introductory organic chemistry courses. **R.M. Kissling**, S. Tong

11:20 CHED **1922.** Probing the origin of student pattern recognition in the organic chemistry classroom. **L.M. McNulty**, **J.J. Esteb**

11:40 CHED **1923.** Using organic chemistry to teach medical diagnosis skills. **M. Ilies**

12:00 Concluding Remarks.

Section F

San Francisco Marriott Marquis

Nob Hill B

Perspectives on Climate Change Literacy & Education: Local to International

Cosponsored by CEI and IAC

K. E. Peterman, *Organizer*

G. P. Foy, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1924.** Geopolitical implications of climate change. **K. O'Keefe**, G.P. Foy, K.E. Peterman

8:55 CHED **1925.** Tackling climate change illiteracy through a space lens. **M. Sobhy**, G.P. Foy, K.E. Peterman

9:15 CHED **1926.** Climate policy at the boundary between science and society. **A.N. Henderson**, G.P. Foy, K.E. Peterman

9:35 CHED **1927.** Indigenous peoples' role in climate change adaptation. **N. Kovil**, G.P. Foy, K.E. Peterman

9:55 CHED **1928.** Energy & sustainability: An introductory course on the intersection of energy, climate, and society. **B. Venkataraman**

10:15 Intermission.

10:25 CHED **1929.** Sustainable food at COP22: Mapping the discussion. **H.P. Melton**, K.E. Peterman, G.P. Foy

10:45 CHED **1930.** Health ramifications of climate change evaluated at the 22nd Conference of Parties (COP22). **T. Yurasits**, K.E. Peterman, G.P. Foy

11:05 CHED **1931.** Climate justice at COP22. **M. Smith**, K.E. Peterman, G.P. Foy

11:25 CHED **1932.** Withdrawn.

11:45 CHED **1933.** Sustainable energy as the focus for a first year seminar. **G.A. Moehring**

12:05 Concluding Remarks.

Section G

San Francisco Marriott Marquis

Nob Hill C

Advancing Undergraduate Research

Research Supportive Curricular Innovations

Cosponsored by PROF

Financially supported by Council on Undergraduate Research

B. L. Gourley, *Organizer*

R. M. Jones, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **1934.** Guided inquiry and drug discovery: A semester-long laboratory sequence for advanced undergraduates. **M.S. Blackledge**, K. Fogarty

8:55 CHED **1935.** Theory and experiment laboratory: Modeling the research experience in a capstone curricular laboratory. **B.L. Gourley**

9:15 CHED **1936.** Research-based organic chemistry laboratory. **M. Bader**, P.T. Pham

9:35 CHED **1937.** Course-Based undergraduate research experience (CURE) in organic chemistry. **L.C. Brown**

9:55 CHED **1938.** Petrochemical incorporation to grow material and characterization bound analytical curriculum: A new attempt to serve dual educational functions. **M. Jiang**

10:15 CHED **1939.** Peptidomimetics from the classroom to the lab: Successful research outcomes from an upper-level class at a primarily undergraduate institute. **D. Guarracino**

10:35 Intermission.

10:50 CHED **1940.** Self-assembly of camptothecin-linked dipeptides. **N.M. Paul**, K.L. Neidrich, K.R. Boggs, A. Shieh, J.R. Parquette

11:10 CHED **1941.** Another round of whiskey for the house: Community college students continue research on experimental new whiskey flavors. **R.L. Silvestri**

11:30 CHED **1942.** Withdrawn.

11:50 CHED **1943.** Leveraging student interest in environmental topics for undergraduate research in an interdisciplinary environmental research cluster. **D.P. Pursell**, K. Zimmermann, N. Khan, S. Park

12:10 CHED **1944.** Developing an interdisciplinary medicinal chemistry undergraduate research program at a small, private, liberal arts university. **J.R. Mays**

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Sponsored by WCC, Cosponsored by CHED, CMA and PROF

Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators

Sponsored by PROF, Cosponsored by BMGT, CHED and PRES

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Environmental Analytical Chemistry

Sponsored by ENVR, Cosponsored by CHED

Processes, Technologies & Sensors for Food-Energy-Water Nexus Research

Sponsored by ENVR, Cosponsored by CEI and CHED

TUESDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Salons 1/2

George C. Pimentel Award in Chemical Education: Symposium to honor Thomas A. Holme

S. Bretz, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1945.** Developing student conceptual understanding in the physical chemistry laboratory. **A. Grushow**, S.S. Hunnicutt, R.M. Whitnell

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

1:55 CHED **1946.** Stability and change: Investigating the blending of mathematics and chemical knowledge in the context of reasoning about chemical kinetics. **M.H. Towns**, K. Bain, A.C. Moon

2:15 CHED **1947.** Adventures in assessment: Moving beyond my students liked it. **J.E. Lewis**

2:35 Intermission.

2:45 CHED **1948.** Holme-made assessment strategies: It would be really neat if. **C.F. Bauer**

3:05 CHED **1949.** ACS Exams Online: Enhanced delivery, scoring and use of ACS Exams. **D. Hart**, K.L. Murphy

3:25 CHED **1950.** ACS Exams: A tradition of excellence in research. **K.L. Murphy**, J.R. Raker

3:45 Intermission.

3:55 CHED **1951. Award Address** (George C. Pimentel Award in Chemical Education sponsored by Cengage Learning & the ACS Division of Chemical Education). Evidence and change, or the lack thereof. **T. Holme**

Section B

San Francisco Marriott Marquis
Salons 3/4

The Role of Research Experiences in the ACS Certified Degree

T. J. Wenzel, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1952.** Role of undergraduate research in the certified chemistry major. **T.J. Wenzel**

1:55 CHED **1953.** Research experiences in the chemistry and biochemistry curriculum at Barnard College: A structure that supports student learning, faculty development, and safety for a diverse population. **R.N. Austin**

2:15 CHED **1954.** Undergraduate research for CPT approval and for preparing minority students for success in PhD programs. **C.G. Gutierrez**, L.M. Tunstad

2:35 CHED **1955.** Five phases for integrating the scientific method and communication skills with research experiences. B. Vernier, M.N. Srnec, A. Carlson, G.A. Buckholtz, E.S. Gawalt, **J.D. Evanseck**

2:55 Intermission.

3:10 CHED **1956.** Improving undergraduate education through innovative research experiences. **N.T. Salzameda**

3:30 CHED **1957.** Starting a research program at primarily undergraduate institution: Practical strategies and supportive policies. **M.L. Kovarik**

3:50 CHED **1958.** Use of active learning pedagogies and undergraduate research experiences to promote student success in chemistry at North Carolina A&T State University. **S.O. Fakayode**, M. Kanipes-Spinks

4:10 CHED **1959.** It's research that makes the Gator chemistry major. **L. McElwee-White**

4:30 Concluding Remarks.

Section C

San Francisco Marriott Marquis
Salon 5

GSSPC: Water Sustainability

Chemists in Pursuit of Clean Water

Cosponsored by CEI and PRES

Financially supported by Georgetown University Department of Chemistry, Graduate Education Advisory Board

Z. De los Santos, J. P. England, Z. Sakhaei, *Organizers*

A. Adcock, I. Brekalo, S. E. Ingram, Z. S. Sakhaei, *Organizers*, *Presiding*

J. Nelson, *Presiding*

1:45 Introductory Remarks.

1:50 CHED **1960.** Role of polymeric structure in reverse osmosis water purification membranes. **B.J. Sundell**

2:20 CHED **1961.** Nanoscale Zero-Valent Iron (nZVI) and iron oxide nanoparticle surface reactions and modification for environmental remediation. **B.E. Koel**

2:50 CHED **1962.** Cactus mucilage: Cleaning water in a sustainable approach. **N. Alcantar**

3:20 Intermission.

3:35 Panel Discussion.

5:05 Concluding Remarks.

Section D

San Francisco Marriott Marquis
Salon 6

Course-Based Undergraduate Research Experiences (CUREs) in Chemistry

R. Waterman, *Organizer*

J. M. Heemstra, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1963.** Student-designed research projects for freshman chemistry majors at UC-Berkeley. **M.C. Douskey**, M.T. Robak, A.M. Baranger, L. Armstrong, G. Kerstiens

1:55 CHED **1964.** Partnership between a two-year transfer program and research faculty to develop a course-based research experience for general chemistry. **K.S. Owens**, A. Murkowski, A.M. Johansen, H. Price, L. Gitelman

2:15 CHED **1965.** Freshman and authentic research, teaching biomedical chemistry through a sequence of course-based research experiences. **S.C. Flynn**, M. Fegley, N. Stamp

2:35 CHED **1966.** Freshman-level research-based laboratories and the transition from student to researcher within the ReBUILDetroit program. **A.L. Feig**, K. Abraham, J. Andreoli, S. Chang, S. Conant, K.R. Evans, A. Fusaro, W. Hao, J. Kagey, G. Kuleck, K.C. Lanigan, A. Mathur, A. Matti, J. Thomson, D. Tomco, S. Welch

2:55 CHED **1967.** Development of a bioinformatics driven research project as an introductory level course-based research experience. **A. Leconte**

3:15 Intermission.

3:30 CHED **1968.** Applying chemical instrumentation in the museum. **K.L. Braun**

3:50 CHED **1969.** Embedding the study of heavy metal water contamination into the analytical chemistry laboratory curriculum. **P. Cleary**

4:10 CHED **1970.** Research in an inorganic laboratory class. **R. Waterman**, J.K. Pagano

4:30 CHED **1971.** Integrating hazard identification and risk assessment into course-based undergraduate research. **S. Sigmann**, D.E. Wheeler

4:50 CHED **1972.** Integrating research opportunities into the inorganic chemistry curriculum at The College of New Jersey. **A.R. O'Connor**, **B.C. Chan**

Section E

San Francisco Marriott Marquis
Nob Hill A

Advances in Teaching Organic Chemistry

S. F. Hornbuckle, *Organizer, Presiding*

1:30 CHED **1973.** Learner-centered approach to teaching undergraduate organic chemistry. **A. Brown**

1:50 CHED **1974.** Teaching organic chemistry with collaborative problem solving in the large lecture setting at UC Berkeley. **M.T. Robak**, A.M. Baranger

2:10 CHED **1975.** Making organic chemistry accessible by promoting student learning through group problem solving. **R. Broyer**

2:30 Intermission.

2:45 CHED **1976.** Deriving of electrostatic potential maps and use of these as a means to predict reactivities between species. **K.K. Bagga**

3:05 CHED **1977.** Evaluation of the relationship between spatial pattern recognition and learning stereochemical principles. **J.J. Esteb**, **L.M. McNulty**

3:25 CHED **1978.** Determination of optical purity of α-methylbenzylamine by formation of the camphor imine: An undergraduate organic chemistry experiment. **S.A. Corlett**, I.F. Germek

3:45 Intermission.

4:00 CHED **1979.** Spectroscopy by the numbers. **N.M. Paul**, C.S. Callam

4:20 CHED **1980.** Back to basics: Improving learning in the organic chemistry laboratory. **A.M. Reeve**

4:40 CHED **1981.** Using analgesics as a corner stone theme for the first semester of Organic Chemistry lecture and lab. R. Blough, **M.J. Castaldi**, **J.K. Murray**

5:00 Concluding Remarks.

Section F

San Francisco Marriott Marquis
Nob Hill B

Writing in Chemistry

S. A. Finkenstaedt-Quinn, *Organizer*

A. C. Moon, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1982.** Faculty practices and beliefs about the effectiveness of writing in promoting student learning in STEM disciplines. **S.A. Finkenstaedt-Quinn**, G.V. Shultz, A. Ruggles Gere

1:55 CHED **1983.** Modification of a junior-level capstone course to incorporate scientific writing. **B. Wile**

2:15 CHED **1984.** Essay writing in the chemistry classroom to enhance learning and raise awareness of social issues affected by chemistry. **A.L. Smalley**, B.R. Fox

2:35 Intermission.

2:50 CHED **1985.** Interactive writing in a two-semester chemical analysis course sequence: Journal-formatted laboratory reports and literature reviews. **R.W. Schaeffer**

3:10 CHED **1986.** Writing-to-learn with Calibrated Peer Review®. **A.A. Russell**

3:30 CHED **1987.** When does this matter in real life? Using chemical knowledge to make fuel choices. **R. Sansom**

3:50 Intermission.

4:05 CHED **1988.** Expanding the students understanding and appreciation of chemistry through reading and writing. **K.K. Bagga**

4:25 CHED **1989.** Use of the science writing heuristic to support instruction aligned to NGSS and the International Baccalaureate's MYP. **N. Hike**, D.J. Wink, **S. Hughes-Phelan**

4:45 CHED **1990.** Development and implementation of a writing-to-learn intervention in introductory quantum mechanics. **A.C. Moon**, E. Zotos, S.A. Finkenstaedt-Quinn, A. Ruggles Gere, G.V. Szymczak

5:05 Concluding Remarks.

Section G

San Francisco Marriott Marquis
Nob Hill C

Advancing Undergraduate Research

Focus on Early Access to Research & Broadening Participation of Under-Represented Groups

Cosponsored by CMA², PROF² and WCC

Financially supported by Council on Undergraduate Research

R. M. Jones, *Organizer*

B. L. Gourley, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **1991.** Undergraduate researchers engaging in chemistry education research. **S.E. Lewis**, R. Oueini, A. Dickerson

1:55 CHED **1992.** Best practices for mentoring undergraduates in international research placements. **J.C. Goeltz**, R.S. Duran

2:15 CHED **1993.** Implementation of the Henderson State University STEM bridge: Challenges and success in the first year. **D. Bateman**, **B.A. Rowland**

2:35 CHED **1994.** Introducing incoming students to research via the Summer Opportunity for Intellectual Activity program. **M.R. Prinsell**, L.J. Moore

2:55 CHED **1995.** FUTURE program: Engaging underserved populations through early research experiences. **A.J. Reig**

3:15 CHED **1996.** Providing early research experiences for undergraduates. **L.J. Silverberg**

3:35 Intermission.

3:50 CHED **1997.** Rethinking the summer research experience for the new majority. **M. Konkle**

4:10 CHED **1998.** Global women and STEM undergraduate research training model. **S. Deprele**

4:30 CHED **1999.** Broadening participation in undergraduate STEM research at the community college. **C.J. Foley**, N. Leonhardt

4:50 CHED **2000.** Leveraging CREST-center funding to advance undergraduate research at multiple Minority Serving Institutions. **K.R. Cousins**, T. Usher, D.C. Smith, R. Zhang, P.K. Dixon

5:10 CHED **2001.** Collaborative field research: A gateway for undergraduate research experiences. **J.C. Ingram**, P. Beamer, K. Chief

Section H

San Francisco Marriott Marquis

Nob Hill D

Simulations, Animations & other Visualizations in Educating about Chemistry SAVE Chemistry!

R. Tasker, *Organizer*

R. M. Kelly, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **2002.** Animation perspectives: Making sense of contrasting molecular animations through commentaries. **R.M. Kelly**

1:55 CHED **2003.** Development of interactive visualizations for use in chemistry courses. **Z. Alghoul**

2:15 CHED **2004.** Simulations in chemistry. **T. Gupta**, G.R. Albing, Z.P. Ziolkowski

2:35 Intermission.

2:50 CHED **2005.** SwissChemCubes - how to play with and use it in classrooms. **M.T. Müller**, A. Togni

3:10 CHED **2006.** Atomarium - 2D- and 3D Visualizations. **M.T. Müller**, A. Togni

3:30 CHED **2007.** Tactile experiences with crystallography to SAVE chemistry! **A. Sarjeant**, P.A. Wood, S. Ward, A.G. Maloney

3:50 CHED **2008.** Augmented reality chemistry: The use of augmented reality to generate 3-D molecular models from 2-D representations. **D. Behmke**

4:10 Intermission.

4:25 CHED **2009.** Using simulations in teaching physical chemistry. **T. Engel**

4:45 CHED **2010.** Illustrating chemical evolution through collaboration with artists. **B.J. McFarland**

5:05 CHED **2011.** Withdrawn.

5:25 Concluding Remarks.

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Source Water Quality

Sponsored by ENVR, Cosponsored by CHED

Science & Perception of Climate Change

Sponsored by ENVR, Cosponsored by CEI and CHED

WEDNESDAY MORNING

Section A

San Francisco Marriott Marquis

Salons 1/2

Using Chemistry Education Research to Inform the Design & Use of Assessment Materials

S. Villafane-Garcia, *Organizer*

J. J. Reed, *Organizer, Presiding*

S. Villafañe, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **2012.** State of assessment use in postsecondary chemistry education. **R. Gibbons**, J.J. Reed, E. Laga, J. Vega, K.L. Murphy, J.R. Raker

8:55 CHED **2013.** Bringing the other elements to shore: Development of the anchoring concept content map for inorganic chemistry. **K.A. Marek**, K.L. Murphy, J.R. Raker, B.A. Reisner

9:15 Intermission.

9:30 CHED **2014.** Encounters with substances: Patterns in chemical identity thinking. **C. Ngai**, H. Sevian

9:50 CHED **2015.** Making predictions and constructing explanations: An investigation into introductory chemistry students' understanding of structure-property relationships. **R. Colvin**, S. Underwood, M. Cooper

10:10 CHED **2016.** Developing assessments to characterize student reasoning about interdisciplinary phenomena. **S.M. Underwood**, E. Scott, C. Anderson, K. Mashood, R. Matz, V. Sawtelle

10:30 Concluding Remarks.

Section B

San Francisco Marriott Marquis

Salons 3/4

Communicating Science in the Twenty-First Century to Diversified Audiences

Cosponsored by CPRC, CWD and PRES

A. E. Neybert, C. A. Supalo, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **2017.** Diversity in communities when communicating science. **D.J. Nelson**

8:55 CHED **2018.** Withdrawn.

9:15 CHED **2019.** Using text-to-speech to provide scaffolding for blind students comprehension of organic chemistry molecular drawings. **A.E. Neybert**, N. TenBroek, C.A. Supalo

9:35 CHED **2020.** Tools of a blind chemist. **M.S. Minkara**

9:55 Intermission.

10:10 CHED **2021.** Science study Includes the blind and visually impaired student. **D. Posont**, F. Wurtzel

10:30 CHED **2022.** Project BLAST: A proactive approach to improving access to science and engineering for blind students. **J. Principato**

10:50 CHED **2023.** Utilizing infographics to advance scientific communication skills. **R.M. Jones**

11:10 CHED **2024.** Teaching students to break down the chemistry of everyday events via infographics. **J.J. Meyers**, **R. Singiser**

11:30 CHED **2025.** Communicating chemical concepts through Braille and other tactile approaches. **H. Wohlers**, C.A. Supalo, L. Walton, C. Wecels, G. Williams

11:50 Concluding Remarks.

Section C

San Francisco Marriott Marquis

Salon 5

Strategies Promoting Success of Two-year College Students

L. J. Anna, T. Higgins, A. M. Palmer, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **2026.** Reaching the hearts and minds of students with case studies and laboratory activities set in local and contemporary contexts. **T.J. Terry**

8:55 CHED **2027.** Developing and implementing open educational resources (OER) for an introductory chemistry course at a two-year community college. **K.J. Smith**

9:15 CHED **2028.** Tool box approach for student success in chemistry. **J.E. Alexander**

9:35 Intermission.

9:50 CHED **2029.** Identifying, recruiting, and motivating undergraduate researchers at a community college through collaboration with the honors program. **D.J. Schauer**

10:10 CHED **2030.** Honors modules to infuse research into the curriculum and enthuse students in chemistry. **L.J. Anna**, A. Palmer

10:30 CHED **2031.** Establishing an ongoing substantive chemistry research program at a two-year college. **C.L. Aronson**, **L.D. Bienski**

10:50 Intermission.

11:05 CHED **2032.** Sharing portable instrumentation to expand instrumentation access and build stronger ties between two-year and four-year institutions. **C.J. Stromberg**, K.H. Bennett, D.J. Ellis, P. Wood, W. Nellis, P. Sheppard, C.A. Bradley

11:25 CHED **2033.** National Science Foundation programs that support chemistry education at community colleges. **T.B. Higgins**, T.D. Kim, D. Rickey

11:45 Concluding Remarks.

Section D

San Francisco Marriott Marquis

Salon 6

Course-Based Undergraduate Research Experiences (CUREs) in Chemistry

J. M. Heemstra, *Organizer*

R. Waterman, *Organizer, Presiding*

8:30 CHED **2034.** Design, synthesis, and evaluation of small molecule sortase inhibitors: A CURE for the undergraduate organic chemistry lab. **J. Antos**, S.A. Reed

8:50 CHED **2035.** CURE for the undergraduate organic chemistry laboratory. **L.M. Stanley**

9:10 CHED **2036.** Discovery-based research using fragment synthesis and protein-observed ^{19}F NMR in an undergraduate organic laboratory. **W.C. Pomerantz**, S. Bur

9:30 CHED **2037.** Leveraging CUREs to increase capacity for traditional undergraduate research experiences and generate student co-authored publications. **J.M. Heemstra**

9:50 CHED **2038.** Known structure, unknown function: A research-based undergraduate biochemistry laboratory course. **L.M. Columbus**, C. Mura, C. Price

10:10 Intermission.

10:25 CHED **2039.** CURE in chemical biology. **P.J. Beuning**

10:45 CHED **2040.** Discovery-based laboratory exercise using the colorful violacein pathway. **J.A. Jones**

11:05 CHED **2041.** Bringing a stress-response research project into the biochemistry laboratory. **R.E. Connor**

11:25 CHED **2042.** Luminescence screening for bioactive compounds: A research-based experiment for undergraduates. **J.A. Prescher**

11:45 CHED **2043.** Taking a new research direction in the Biochemistry II teaching lab. **B.J. McFarland**

Section E

San Francisco Marriott Marquis

Nob Hill A

Research in Chemistry Education

D. P. Cartrette, D. R. Mulford, *Organizers*

M. Mack, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **2044.** Influence of an international field research experience on high school teachers' understandings of the practices of science and engineering. **M. Orgill**, J. Adams, S. Nealy, C. Kardash

8:55 CHED **2045.** Evolution of high- and low-achieving students' knowledge structures over general chemistry courses. **O. Gulacar**, M. Seibel, B. Kung, A. Milkey, S. McLane

9:15 CHED **2046.** Evaluating students' awareness of and attitudes toward scientific research at a public, open-access college. **M. Anzovino**

9:35 CHED **2047.** Students' understanding of energy in chemical reactions and processes. **K. Bain**, H. Hamby, T. McCord, M.H. Towns

9:55 Intermission.

‡ *Cooperative Cosponsorship*

10:10 CHED **2048.** Exploring learning outcomes when using multimedia for chemistry reaction mechanisms. **A. Bongers**, A.B. Flynn

10:30 CHED **2049.** Peeking inside the black box: Making learning visible using an ethnographic perspective. **L. Fallot**, M.Z. Kalainoff, E.M. Kowalski

10:50 CHED **2050.** Patterns of reactions: A card sort task to explore students' connections across organic chemistry reactions. **K.R. Galloway**, M.W. Leung, A.B. Flynn

11:10 Concluding Remarks.

Section F

San Francisco Marriott Marquis

Nob Hill B

Undergraduate Laboratory Experiments Involving Advanced Materials

Cosponsored by MPPG‡

W. J. Miller, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **2051.** Laboratory experiments making applied materials. **G. Lisensky**

9:20 CHED **2052.** Introducing green and nongreen aspects of noble metal nanoparticle synthesis: An inquiry-based laboratory experiment for chemistry and engineering students. **I.E. Pavel Sizemore**, S. Paluri, M. Newsome

9:40 Intermission.

9:55 CHED **2053.** Introduction of galvanic replacement reactions at the nanoscale to undergraduate students: Synthesis of hollow metal nanostructures. **J. Chen**

10:15 CHED **2054.** Quantifying gold nanoparticle concentration in suspensions using smartphone colorimetry. C. Knutson, A.R. Campos, T.R. Knutson, A.R. Mozzetti, C.L. Haynes, **R. Penn**

10:35 CHED **2055.** Undergraduate laboratory experiment modules for probing gold nanoparticle interfacial interactions. **D. Zhang**

10:55 Intermission.

11:10 CHED **2056.** Introducing undergraduates to functionalizing nanoparticle surfaces for solar cell applications. **J. Zemke**

11:30 CHED **2057.** Fabrication and characterization of solution processed perovskite solar cells by undergraduates at California State University, Chico. **M.C. So**, J. Barnett, V. Cherrette, C. Hutcherson

11:50 CHED **2058.** Investigating bandgap energies, materials, and design of light-emitting diodes. **E.P. Wagner**

12:10 Concluding Remarks.

Section G

San Francisco Marriott Marquis

Nob Hill C

Advancing Undergraduate Research

Cosponsored by CMA, PROF and WCC

Financially supported by Council on Undergraduate Research

R. M. Jones, *Organizer*

B. L. Gourley, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **2059.** Senior undergraduate research and assessment at Florida Southern College. **D.C. Bromfield-Lee**, A. Le

8:55 CHED **2060.** Innovative undergraduate research program at Tennessee Tech. **E.C. Lisic**

9:15 CHED **2061.** Undergraduate research in STEM fields at Georgia Southern University: A fifteen-year prospective from a former program director. **M. Davis Mcgibony**

9:35 CHED **2062.** Transformative impact of developing and implementing a comprehensive undergraduate research program. **B.E. Holmes**, G.L. Heard

9:55 CHED **2063.** Assessing undergraduate research in chemistry: A comparison study. **R.M. Jones**

10:15 CHED **2064.** Using undergraduate research to enhance STEM education at the institutional and system-wide level. **M.R. Malachowski**, K.K. Karukstis, J. Osborn, E. Ambos

10:35 Intermission.

10:50 CHED **2065.** Organizing, assessing, and enriching undergraduate research experiences. **K.D. Schurmeier**

11:10 CHED **2066.** Dreams, realities and strong contributions to diversity in STEM: Impact of an undergraduate research office at a Hispanic serving institution. **L.E. Echegoyen**, L. Diaz-Martinez, G. Corral

11:30 CHED **2067.** Using case studies to understand undergraduate research experiences. **S.L. Johnson**, G.M. Bodner

11:50 CHED **2068.** Investigation of learning outcomes from undergraduate research experiences. M.R. Helix, L.E. Cote, E.M. Stone, **A.M. Baranger**

12:10 Discussion.

12:25 Concluding Remarks.

Section H

San Francisco Marriott Marquis

Nob Hill D

Research on Learning in the Lab

Cosponsored by IAC‡

M. J. Chrzanowski, S. Sandi-Urena, *Organizers*

S. Sandi-Urena, *Presiding*

8:30 Introductory Remarks.

8:35 CHED **2069.** Withdrawn.

8:55 CHED **2070.** Scenarios as a tool for investigating risk perception in the general chemistry laboratory. **S. Haxton**, S.D. Wiediger

9:15 CHED **2071.** Analysis of diverse and independent laboratory learning environments using Langer's mindfulness theory. **E. Jimenez Alvarado**, **S. Sandi-Urena**

9:35 Intermission.

9:50 CHED **2072.** Impact of nature of science instruction on the chemistry laboratory experience. **G. Kerstiens**, A.M. Baranger, M.C. Douskey, M.T. Robak, L. Armstrong

10:10 CHED **2073.** Investigating the effect of a project-based laboratory curriculum on students' value of science. **J.H. Carmel**, J.S. Ward, A. Pollock, L.A. Posey, M. Cooper

10:30 CHED **2074.** Exploring metacognitive activity in a collaborative third year organic chemistry laboratory. **K. Mathabathe**, M. Potgieter, M. Rollnick

10:50 CHED **2075.** Learning in the tertiary level chemistry laboratory: Findings from phenomenology research. **M.J. Chrzanowski**, **S. Sandi-Urena**

11:10 Concluding Remarks.

Active Learning in the Undergraduate Analytical Chemistry Curriculum

Sponsored by ANYL, Cosponsored by CHED

WEDNESDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Salon 1/2

Using Chemistry Education Research to Inform the Design & Use of Assessment Materials

S. Villafane-Garcia, *Organizer*

J. J. Reed, *Organizer, Presiding*

S. Villafañe, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **2076.** Fidelity of implementation: An overlooked construct in chemical education research. **M.N. Stains**

1:55 CHED **2077.** Assessment of process skills in student responses to open-ended exam questions. **J.A. Schmidt-McCormack**, R.S. Cole, C. Fish, A.M. Falke, J. Lantz

2:15 CHED **2078.** Community-produced assessment instrument for biochemistry: Linking research and practice. **J.A. Loertscher**, J.E. Lewis, A. Mercer, V.M. Thorsell

2:35 Intermission.

2:50 CHED **2079.** Response process validity study for a cross-disciplinary assessment. **J.M. Trate**, V. Fisher, A. Blecking, P. Geissinger, K.L. Murphy

3:10 CHED **2080.** Evaluating the psychometric evidence of the approaches to teaching inventory and the implications for psychometrics in chemistry education research. **J. Harshman**, M.N. Stains

3:30 Concluding Remarks.

Section B

San Francisco Marriott Marquis

Salon 3/4

Communicating Science in the Twenty-First Century to Diversified Audiences

Cosponsored by CPRC, CWD and PRES

A. E. Neybert, C. A. Supalo, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **2081.** Auxiliaries of wisdom: Challenges of science education at an Orthodox Jewish College. **J.M. Newman**

1:55 CHED **2082.** Developing and advocating for non-visual techniques in general and organic chemistry. **E.D. Schlenker**

2:15 CHED **2083.** Chemistry a la CART: Making chemistry accessible for d/Deaf and hard of hearing. **M.A. Postlewaite**

2:35 CHED **2084.** Developing hands-on learning modules for blind and visually impaired high school and undergraduate chemistry students. **R. Dabke**, S. Melaku, J. Schreck, Z. Gebeyehu, K.K. Griffin

2:55 Intermission.

3:10 CHED **2085.** Creation and assessment of a concept-based chemistry curriculum. **P.K. Morehouse**

3:30 CHED **2086.** Game-based learning in chemistry. **T. Gupta**, G. Albing, J. Rosenbaum

3:50 CHED **2087.** Service dogs in the chemistry laboratory. **P.A. Redden**

4:10 CHED **2088.** Bridging the Sino-American divide in green chemistry: A parable of overcoming activation barriers in language, creeds, philosophies, diversity, and handicaps. **L.A. Lucia**

4:30 CHED **2089.** Signaling safety in the chemistry classroom. **A.A. Eroy-Reveles**, J. Nagy, M. Estrada

4:50 Concluding Remarks.

Section C

San Francisco Marriott Marquis

Salon 5

Strategies Promoting Success of Two-year College Students

L. J. Anna, T. Higgins, A. M. Palmer, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **2090.** Student affective state and reading ability: Implications for prerequisites and instruction in introductory and general chemistry classes. **J. Ross**, C. Lai, L. Nuñez

1:55 CHED **2091.** Impact of in-class calculation work-sheet in chemistry and physical science courses on student success. **G. Gyanwali**

2:15 CHED **2092.** Rules for success for teachers and students in a two-year college. **M.J. Kenney**

2:35 Intermission.

2:50 CHED **2093.** Strategies for overcoming significant challenges faced by the two-year college student. **D. Lewis**, **L. Louis**, **J.L. Sams**, **A.J. Sanders**

3:10 CHED **2094.** Opening doors to STEM teaching with a learning assistant program. **C.P. Schick**

3:30 CHED **2095.** NSF scholarship programs for community college students and minority serving institutions. **T.B. Higgins**, T.D. Kim, D. Rickey

3:50 Concluding Remarks.

Section D

San Francisco Marriott Marquis

Salon 6

Course-Based Undergraduate Research Experiences (CUREs) in Chemistry

R. Waterman, *Organizer*

J. M. Heemstra, *Organizer, Presiding*

1:30 CHED **2096.** Incorporating research-like experiences in a physical chemistry for the life sciences course. **J.G. Rowley**

1:50 CHED **2097.** Integrating paper microfluidics research into the undergraduate curriculum: CUREs at Cal State LA. **F.A. Gomez**, W. Lee, K. Parducho

2:10 CHED **2098.** Drugs and cells: A cross-disciplinary, medicinal chemistry laboratory course. **T.W. Funk**, J. Brandauer

2:30 CHED **2099.** Distributed drug discovery experiments in undergraduate organic chemistry laboratories. **W.L. Scott**, **A.A. Fuller**, A.B. Dounay, M. O'Donnell, J.G. Samaritoni

3:10 Intermission.

3:30 CHED **2100.** Two-photon absorption spectroscopy on curcumin in solution: A state-of-the-art physical chemistry experiment. **J. Donnelly**, F. Hernandez

3:50 CHED **2101.** Superlab: Junior-year integrated laboratory at Haverford College. **C.H. Londergan**

4:10 CHED **2102.** Bringing the outdoors in: A multi-institution, multi-course, collaborative effort to integrate water quality projects into laboratory curricula. **T. Sivy**, A. Lukowski, E.M. Greeson, J. Tomasik

4:30 CHED **2103.** Integrated research lab at Guilford College: A course-based research experience for organic, inorganic, and physical chemistry students. **A.G. Glenn**, G.H. Webster, R.M. Whitnell

4:50 Concluding Remarks.

Section E

San Francisco Marriott Marquis
Nob Hill A

Research in Chemistry Education

D. P. Cartrette, D. R. Mulford, *Organizers*

R. Komperda, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **2104.** Effect of self-explaining on scientific-skill development: Longitudinal study via latent transition analysis. **A. Villalta-Cerdas**

1:55 CHED **2105.** Persistence in STEM: Development of a longitudinal model integrating self-efficacy, outcome expectations and performance in chemistry gateway courses. **S. Srinivasan**, K.L. Murphy

2:15 CHED **2106.** Roles of personal and contextual factors in the characterization of the impact of the Cottrell Scholars Collaborative New Faculty Development Workshop. **J. Harshman**, M.N. Stains

2:35 Intermission.

2:50 CHED **2107.** Anxiety and enjoyment: Exploring students' academic emotions in general chemistry. **S. Villafane-Garcia**, X. Xu, J.R. Raker

3:10 CHED **2108.** Describing student experiences in a project-based organic chemistry laboratory. **N.L. Burrows**, S.R. Mooring

3:30 CHED **2109.** Withdrawn.

3:50 Concluding Remarks.

Section F

San Francisco Marriott Marquis
Nob Hill B

Undergraduate Laboratory Experiments Involving Advanced Materials

Cosponsored by MPPG‡

W. J. Miller, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **2110.** Raman microscopy study of graphene: An upper-level undergraduate experiment. **H. Liu**, M.M. Ward

1:55 CHED **2111.** Fabrication of polyvinylpyrrolidone micro-/nanostructures utilizing microcontact printing. **W.C. Sanders**

2:15 CHED **2112.** Low-catalyst concentration atom transfer radical polymerization in the undergraduate laboratory: Synthesis of well-defined epoxide-containing polymers and their postpolymerization modification to fluorescent materials. **N.V. Tsarevsky**, S.R. Woodruff, P. Wisian-Neilson

2:35 Intermission.

2:50 CHED **2113.** Withdrawn.

3:10 CHED **2114.** Colorimetric anion sensing in undergraduate analytical chemistry. **M.O. Odago**

3:30 CHED **2115.** Solvent-water-partitioning of different pH-indicators: A classroom and a self-experiencing laboratory sequence. **M.T. Müller**, B. Escher

3:50 Intermission.

4:05 CHED **2116.** Analysis of metal oxide and organic UV absorbers in commercial sunscreens. **R. Quinones**

4:25 CHED **2117.** It does rain in Southern California. **J. Ashcroft**, B. Last, R. Ehrmann, A. Cakmak, E. Bautista

4:45 CHED **2118.** Simple experiment to introduce nanophytotoxicity to first-year undergraduate students. S. Ross, M. Owen, B. Pedersen, G. Liu, **W.J. Miller**

5:05 Concluding Remarks.

Section G

San Francisco Marriott Marquis
Nob Hill C

Eliciting Attentiveness from Cyber-Savvy Students without Using Electronic Tools

K. Kostecka, *Organizer*

C. E. Cannon, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHED **2119.** Old school teaching (and learning!). **P.F. Brandt**

1:55 CHED **2120.** Facilitating the formation of an e-free classroom community: A chemistry classroom exercise. **B. Budy**

2:15 CHED **2121.** Course Preparation Assignments as a teaching tool in one-semester undergraduate biochemistry courses. **N.J. Ronkainen**

2:35 CHED **2122.** Sneaking in the science. **P.A. Redden**

2:55 CHED **2123.** Discussions during lecture in a large-enrollment chemistry course and during lab in a small-enrollment tribal college chemistry course. **M.A. Griep**, B. DeVore-Wedding

3:15 Intermission.

3:30 CHED **2124.** Physical presence and chemistry of art, color, and artifact conservation. **M.J. Welsh**

3:50 CHED **2125.** Short writes and journals as effective teaching tools in nutritional chemistry. **C.E. Cannon**

4:10 CHED **2126.** Science and science fiction in the classroom. **D.A. Katz**

4:30 CHED **2127.** Use of science and science fiction based television and movie clips in the instruction of non-chemistry majors. **K. Kostecka**

4:50 Concluding Remarks.

Section H

San Francisco Marriott Marquis
Nob Hill D

General Papers

S. A. Fleming, *Organizer*

V. Feng, *Presiding*

1:30 Introductory Remarks.

1:35 CHED **2128.** Determination of the overall antioxidant strength of teas combining metal nanoparticles, plasmonics, and fluorescence: Designing new experiments for the physical chemistry laboratory. **J. Donnelly**, F. Hernandez

1:55 CHED **2129.** Fluorescent carbon dots: A new material to teach nanotechnology throughout chemistry curriculum. **V. Feng**, J. Kuether, R. Tapia Hernandez, S.N. Pham, B. Zhi, M. Krause, C.L. Haynes

2:15 CHED **2130.** Fine-grained analysis of general chemistry texts' treatment of rates of change concepts in reaction kinetics. **S. Seethaler**, J. Czworkowski, L. Wynn

2:35 Intermission.

2:50 CHED **2131.** Guided inquiry experiment involving the intrinsic viscosity of a polymer in aqueous solution. **A.L. Marsh**

3:10 CHED **2132.** Determination of essential minerals and toxic elements in Aggie Farm produce by ICP-OES: A problem based and guided inquiry learning experience in instrumental analysis laboratory course. **S.O. Fakayode**, N. Nickolas, L. Hordge, T. Jackson, D. Keyes, M. Duncan

3:30 CHED **2133.** Withdrawn.

3:50 CHED **2134.** Design of a rime-of-flight secondary ion mass spectrometer for hands-on undergraduate instruction. **M.V. Lee**

Active Learning in the Undergraduate Analytical Chemistry Curriculum

Sponsored by ANYL, Cosponsored by CHED

WEDNESDAY EVENING

Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences

Sponsored by ENVR, Cosponsored by ANYL and CHED

Science & Perception of Climate Change

Sponsored by ENVR, Cosponsored by CEI and CHED

THURSDAY MORNING

Section A

San Francisco Marriott Marquis
Sierra A

How Do We Teach Collaboration? Best Practices for Educating Future Researchers & Innovators

Cosponsored by CHED

Financially supported by NSF Centers for Chemical Innovation

B. Hames, M. Krause, D. Watt, *Organizers*

M. DeBoever, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 CHED **2135.** Outreach as a cross-disciplinary collaboration: Design and implementation of an interactive aerosol chemistry display. **H. Weizman**, **B. Hames**

8:30 CHED **2136.** Weaving chemistry, biology, and microbiology labs into common themes: Illustrating relevance across disciplines. **K.V. Waynant**, D. Felton, P. Hartzell, M. Ederer

8:50 Intermission.

9:00 CHED **2137.** Review on training undergraduate and graduate students to conduct interdisciplinary research. **R.Y. Lai**, **P. Dussault**, M. Schubert, A.E. Holmes

9:20 CHED **2138.** Postdoctoral training within Nebraska MRSEC: A review. **R.Y. Lai**, J. Bosley

9:40 CHED **2139.** Beyond the bench: Educating students in collaborative, innovative team science. **J.M. Amador**, M. Dolgos, D.A. Keszler, J.C. Giordan

10:00 Intermission.

10:10 CHED **2140.** Keys to successful collaboration: Insights from the Centers for Chemical Innovation. M. DeBoever, B. Hames, **M. Krause**, D. Watt

Section B

San Francisco Marriott Marquis
Sierra B

Current Best Practices for Chemistry REU Programs

Cosponsored by PRES

M. A. Griep, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CHED **2141.** Coordination of the chemistry REU program at the University of Nebraska-Lincoln. **M.A. Griep**

8:25 CHED **2142.** How a partnership model for REU programs can lead to chemistry careers for underserved students. **J.B. Halpern**, S. Sinex, P. Sabila

8:45 CHED **2143.** Summer International REU Program in the United Kingdom: Successes, challenges and best practices. M. Crowe, **A.G. Glenn**, **T.A. Nile**

9:05 CHED **2144.** Summer REU program integrating deaf and hearing participants in chemistry research. **K.L. Caran**, G. MacDonald

9:25 Intermission.

‡ *Cooperative Cosponsorship*

9:40 CHED **2145.** Mutli-Institution REU site on environmental/green chemistry. **J.A. Rice**, D. Asunskis, G.P. Nora

10:00 CHED **2146.** We can work(shop) it out: Benefits of technical workshops to REU programs. **M.W. Peczuh**, J. Gascon, C. Bruckner, G.A. Crundwell

10:20 CHED **2147.** Providing laboratory safety education to REU audiences. **R. Stuart**, S.B. Sigmann

10:40 Concluding Remarks.

Section C

San Francisco Marriott Marquis
Sierra C

Engaging Students in Physical Chemistry

Cosponsored by PHYS

C. M. Teague, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CHED **2148.** Development of a guided inquiry experiment on symmetry and spectroscopy. **C.M. Teague**

8:55 CHED **2149.** Measuring the speed of sound and heat capacity ratio of gases by acoustic interferometry: A physical chemistry laboratory experiment. **T.D. Varberg**, B.W. Pearlman, I.A. Wyse, K.L. Moffett

9:15 CHED **2150.** Incorporating science writing into the physical chemistry laboratory course. **A.M. Fleshman**

9:35 CHED **2151.** Incorporating research projects into an undergraduate physical chemistry laboratory course. **M. Wilker**

9:55 Intermission.

10:10 CHED **2152.** Connecting the dots in physical chemistry survey using narrative and authentic research. **B.J. McFarland**

10:30 CHED **2153.** Learning physical chemistry through data analysis. **J. Selco**

10:50 CHED **2154.** Engaging students in connecting representational levels for better understanding of thermodynamics. **R.S. Cole**, C. Stanford, A.C. Moon, M.H. Towns

11:10 CHED **2155.** Development of foundational and in-depth guided inquiry activities for physical chemistry. **A.L. Marsh**

11:30 Concluding Remarks.

Section D

San Francisco Marriott Marquis
Sierra H

Instructors & Researchers: Advancing Graduate Student Education

G. Bhattacharyya, S. J. Hansen, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 CHED **2156.** Fighting the battle to disconnect science education with the descriptor K-12. **G.M. Bodner**

8:25 CHED **2157.** Becoming a graduate student in chemistry as a blind learner: Surfacing interventions for success from an autoethnographic case. **C.A. Supalo**

8:45 CHED **2158.** Guiding career planning and preparation: ACS development of Individual Development Plan (IDP) resources. **C.Y. Kuniyoshi**, **J.L. Wesemann**, N.S. Goroff, N. Bakowski

9:05 CHED **2159.** Withdrawn.

9:25 Intermission.

9:40 CHED **2160.** Community: Promoting the success of students of color in graduate programs. **L. Winfield**, K.M. Jackson

10:00 CHED **2161.** Enhancing graduate education and broadening participation at Louisiana State University through LA-BRIDGE. **G. Thomas**, Z.S. Wilson-Kennedy, I.M. Warner, A. Wright

10:20 CHED **2162.** Withdrawn.

10:40 CHED **2163.** Discipline-specific graduate course on teaching methods: Cultivating change agents in chemical education. **S. Brydges**, H. Dembinski, M. Boerneke, K. Finzel, C. Weinstein, R. Peacock

11:00 Concluding Remarks.

Section E

San Francisco Marriott Marquis
Sierra I

General Papers

S. A. Fleming, *Organizer*

M. L. Curry, *Presiding*

8:00 Introductory Remarks.

8:05 CHED **2164.** Withdrawn.

8:25 CHED **2165.** Improving scientific communication skills in students through professionalism in chemistry II. **S. Gamagedara**

8:45 CHED **2166.** What is the real cost of contingent faculty? Evaluation of the impact of teaching professionals on undergraduate socialization. **K. Van Kirk**

9:05 CHED **2167.** Promoting STEM education through an early STEM college hands-on research internship experience. **S.O. Fakayode**, J. Tinsley, V. Abiera, D. Mehta, J. Smith, N. Whitehead, B. Elzey, E. Appah

9:25 Intermission.

9:40 CHED **2168.** Molecular modeling across the undergraduate curriculum. **T. Madison**, **E.P. Wagner**

10:00 CHED **2169.** Reciprocal peer tutoring in general chemistry: Benefits to information retention and lowered student test anxiety. **D.W. Carpenetti**

10:20 CHED **2170.** Design and implementation of an undergraduate peer-learning program at UC Berkeley. **P. Marsden**, M.T. Robak, A.M. Baranger, S. Tischhauser

10:40 CHED **2171.** Research Experiences for Teachers (RET) site: Sustainable electronics. A.L. Curry, I. Hua, **M.L. Curry**

Section F

San Francisco Marriott Marquis
Sierra J

General Papers

S. A. Fleming, *Organizer*

J. E. Owens, *Presiding*

8:00 Introductory Remarks.

8:05 CHED **2172.** Illuminating the photoredox-catalyzed Chan-Lam coupling reaction: Building understanding of a modern organic synthesis method. J. Marshall, P.M. Lundin, M.S. Blackledge, **A.J. Wommack**

8:25 CHED **2173.** Using the Suzuki-Miyaura reaction to introduce organic chemistry laboratory students to reaction development of a pharmaceutically active compound. **P.M. Lundin**

8:45 CHED **2174.** Detecting olive oil adulteration: A senior research project. **R. Indralingam**, C.T. Michael

9:05 CHED **2175.** Combining coffee bean trace element profiles and origins as sources of data for teaching principle component analysis. **C.J. Taylor**

9:25 Intermission.

9:40 CHED **2176.** Team-based learning in two upper-division chemistry elective courses: Mass spectrometry and environmental chemistry. **J.E. Owens**

10:00 CHED **2177.** Calculating charge densities for solvatochromic dyes: A computational chemistry project for the physical chemistry curriculum. **B. Findley**, T.F. Nedder

10:20 CHED **2178.** Identifying student misconceptions and analyzing student thought processes during construction and application of molecular orbital diagrams. A.D. Spurlock, **J.L. Jenkins**

10:40 CHED **2179.** Guided inquiry approach to understanding fluorescence spectroscopy. **M.P. Hill**, E. Nam

Section G

San Francisco Marriott Marquis
Sierra K

General Papers

S. A. Fleming, *Organizer*

S. M. Tremain, *Presiding*

8:00 Introductory Remarks.

8:05 CHED **2180.** Elemental nucleogenesis is made simple with cartoon drawings of the quarks making hydrogen's protons and neutrons continuing on in heavier elements showing interesting trends in the chart of the nuclides. **R.J. Schroeder**

8:25 CHED **2181.** Reinforcing the foundations of chemical knowledge. **K.D. Revell**

8:45 CHED **2182.** How to maximize class time and bridge learning gaps using just-in-time-teaching. **R. Glazener**

9:05 CHED **2183.** Using student group presentations in biochemistry for program level assessment. **S.M. Tremain**

9:25 Intermission.

9:40 CHED **2184.** Using a shortened periodic table to teach general chemistry. **M.J. Kenney**

10:00 CHED **2185.** Preparation and characterization of cobalt coordination complexes: An advanced inorganic laboratory project. **W.A. Neiwert**

10:20 CHED **2186.** Withdrawn.

10:40 CHED **2187.** Teaching atomic structure as a threshold concept in chemistry for biologists. **E. Loizidou**, H. Jones

Section H

San Francisco Marriott Marquis
Sierra E

The General Chemistry Course for a Changing World

D. A. Katz, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 CHED **2188.** Steps toward integrating the general chemistry course. **D.A. Katz**

8:25 CHED **2189.** General chemistry pedagogy to engineering students *via polymer structure-property relationships*. **C.L. Aronson**, **R. Muzquiz**, **L.D. Bienski**

8:45 CHED **2190.** Withdrawn.

9:05 Intermission.

9:20 CHED **2191.** Adaptive learning: Reflections and indications. **E.C. Gravely**, G.P. Redd, T.C. Redd

9:40 CHED **2192.** Some considerations for teaching general chemistry in the global communities of the second machine age. **C.A. Supalo**

10:00 CHED **2193.** Pathways to success in general chemistry. **K.L. Stone**, **S.E. Shaner**, C.M. Fendrick

10:20 CHED **2194.** Introductory chemistry through social contexts. **B. Venkataraman**

10:40 Concluding Remarks.

How Do We Teach Collaboration? Best Practices for Educating Future Researchers & Innovators

Cosponsored by CHED

CHAS

Division of Chemical Health and Safety

D. Decker, *J. Pickel and F. Wood-Black, Program Chairs*

SUNDAY MORNING

Nanocellulose Processing & Analysis

Novel Processes

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

SUNDAY AFTERNOON

Section A

Park Central San Francisco
Olympic

Best Practices in Selecting & Presenting Safety Training Content

Cosponsored by CCS and PRES

D. M. Decker, F. K. Wood-Black, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 CHAS **1.** Connecting safety culture to the educational mission. **R. Stuart**

1:55 CHAS **2.** Preliminary results of the chemical safety information and education survey. **E. Sweet**

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

2:15 CHAS **3.** Building safety culture through targeted training. **M.R. Wilhelm**

2:35 CHAS **4.** Flipped classroom techniques in safety training. **R.M. Izzo**

2:55 CHAS **5.** Relevant content, positive attitude, and memorable presentation. **K.P. Fivizzani**

3:15 Concluding Remarks.

Section A

Park Central San Francisco

Olympic

Ask Dr. Safety: Chemical & Occupational Safety in the Cannabis Industry

Cosponsored by CCS

H. J. Elston, N. R. Langerman, *Organizers*, *Presiding*

3:35 Introductory Remarks.

3:40 CHAS **6.** Sensible approach to workplace drug testing for cannabis. **J. Marcu**, R.W. Phifer, E.M. Pryor

4:00 CHAS **7.** Ask Dr. Safety: Chemical & occupational safety in the cannabis industry. **N.R. Langerman**, H.J. Elston

Nanocellulose Processing & Analysis

Process Parameters

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

MONDAY MORNING

Section A

Park Central San Francisco

Olympic

Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing

Cosponsored by CCS and SCHB‡

J. Marcu, E. M. Pryor, *Organizers*, *Presiding*

9:00 Introductory Remarks.

9:05 CHAS **8.** Cannabis analysis: An overview of testing requirements and challenges in a rapidly emerging industry. **M.J. Wilcox**, J. Marcu

9:25 CHAS **9.** Quality control analysis of contaminants in the medical cannabis market in California: Pesticide, plant growth regulators, residual solvents, and microbiological contaminants in cannabis, cannabis extracts, and cannabis infused products. **J. Wurzer**

9:45 CHAS **10.** States as cannabis laboratories: The far-reaching implications of federal non-recognition in the regulation of marijuana contaminants. **J. Angermann**, J. Strull

10:05 Intermission.

10:20 CHAS **11.** Assessing regulatory compliance at medical cannabis operations in the United States for patient focused certification. **J. Marcu**, K. Nevedal, S. Sherer

10:40 CHAS **12.** Challenges cannabis laboratories face in product analysis representative samples. **D. Chen**

11:00 CHAS **13.** Hemp as a nutritional supplement: Ensuring potency, safety, and regulatory compliance in manufacturing cannabis-derived health products. **A. Pham**

11:20 Concluding Remarks.

Nanocellulose Processing & Analysis

Properties

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

MONDAY AFTERNOON

Section A

Park Central San Francisco

Olympic

Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing

Cosponsored by CCS and SCHB‡

J. Marcu, E. M. Pryor, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 CHAS **14.** Residual solvent contaminants in cannabis concentrates. **J.T. Fischedick**, D. Egerton

1:55 CHAS **15.** Cannabis grow facilities: Identification and handling of hazardous wastes, a problem for Environmental Health Departments. **D. Keenan**, M. Duazo

2:15 CHAS **16.** Thermal decomposition of THC on preparation of a distilled hash oil: A case study. **D. Lane**

2:35 Intermission.

2:50 CHAS **17.** THCA and CBDA: More than simply inactive precursors. **G. Moreno**

3:10 CHAS **18.** Emerging challenges in cannabis regulations. **R. Mirkarimi**

3:30 CHAS **19.** CANN History: The first year as a subdivision at the ACS. E.M. Pryor, **J. Marcu**, M.J. Wilcox, E.L. Oltermann, A. Pham

3:50 Panel Discussion.

Nanocellulose Processing & Analysis

Fundamentals

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

J. M. Pickel, *Organizer*

8:00 - 10:00

CHAS **20.** Perception of risk in a quantitative analytical teaching laboratory. **S. Haxton**, S.D. Wiediger

CHAS **21.** Absence of safety education in chemistry curriculum, and *Normalization of Deviance*. **R.H. Hill**

CHAS **22.** Revisiting and revising The Safety Ethic. **R.H. Hill**

CHAS **23.** Assessing risk for undergraduate research and demonstrations. **R. Stuart**, S.B. Sigmann

CHAS **24.** Division of Chemical Health and Safety information poster. **J.M. Pickel**

CHAS **25.** Cannabis analysis: A complex job under complex circumstances. **M.J. Wilcox**, J. Marcu

CHAS **26.** Implementing sustainable practices in hands-off academic research labs. **K.A. Miller**

CHAS **27.** Safety as a core value of a student chapter. **C. Wilhelm**

CHAS **28.** Improving the safety culture of the University of California, Irvine through a graduate safety fellowship. **T. Endean**

CHAS **29.** Assessing secondhand marijuana smoke using biological markers. **B. Wei**, L. Wang

TUESDAY MORNING

Section A

Park Central San Francisco

Olympic

Information Flow in Environmental Health & Safety

Cosponsored by CCS and CINF‡

R. Stuart, *Organizer, Presiding*

9:00 Introductory Remarks.

9:10 CHAS **30.** Chemical safety requires a system, not a solution. **R. Stuart**

9:35 CHAS **31.** Chemical information necessary to establish laboratory ventilation control bands. **E. Sweet**

10:00 CHAS **32.** Reaction safety information: Engaging the community in collecting and sharing of safety learnings. **C. Nitsche**, G. Whittick, M. Manfredi

10:25 Intermission.

10:35 CHAS **33.** Chemical management applications for the University of California. **P. Painter**, C. Carcamo

11:00 CHAS **34.** Comparing GHS hazard statements between different sources. B.S. Clark, B. Murphy, P.D. Tran, D. Berleant, R. Stuart, **R.E. Belford**

11:25 CHAS **35.** Talking chemical safety: Terminologies and keywords in various information sources. **L. McEwen**

11:50 Panel Discussion.

TUESDAY AFTERNOON

Section A

Park Central San Francisco

Olympic

Information Flow in Environmental Health & Safety

Cosponsored by CCS and CINF‡

R. Stuart, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CHAS **36.** Consult the SDS. **S. Sigmann**

2:00 CHAS **37.** Graduate student perspective on the ACS online tool Hazard Assessment in Research Laboratories. **K. Leahy**

2:25 CHAS **38.** Unique one-stop access to a multitude of chemical safety resources. **A. Lederman**

2:50 Intermission.

3:05 CHAS **39.** EPA CompTox chemistry dashboard: An online resource for environmental chemists. **A.J. Williams**, C. Grulke, J. Smith, K. Mansouri, A. McEachran, K. Dionisio, K. Phillips, G. Patlewicz, J. Fitzpatrick, T. Martin, A. Richard, J. Edwards

3:30 CHAS **40.** Exposure driven risk assessment of nanoparticles: Towards a re-equilibration of the traditional risk = hazard x exposure equation. **A. Mason**, C. de Garidel-Thoron, S. Pekar, M. Auffan, J. Rose, M. van Tongeren, P.K. Westerhoff

3:55 CHAS **41.** Assessing the activity and toxicity profile of small-molecules using freely accessible software and data: The contributions of chemical ontologies, metabolism prediction, and spectra prediction. **Y. Djoumbou Feunang**

Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce

Sponsored by CHAL, Cosponsored by CHAS, ENVR and I&EC

WEDNESDAY MORNING

Section A

Park Central San Francisco

Olympic

What Have We Learned & Where Are We Going: Post-Settlement in the University of California

Cosponsored by CCS and PRES

D. M. Decker, J. Palmer, *Organizers*, *Presiding*

9:00 Introductory Remarks.

9:05 CHAS **42.** Moving from compliance to safety in UC laboratories. **C.A. Merlic**

9:30 CHAS **43.** 2700 Miles and a big step forward: The UC settlement and Princeton University. **R.M. Izzo**

9:55 CHAS **44.** Beyond compliance: Building safety culture at UCLA. **C. Dimock**, **S. Hsieh**

10:20 Intermission.

10:35 CHAS **45.** Moving on after the settlement - the approach of a small University of California campus. **K. Smith**

11:00 CHAS **46.** Continuous improvement opportunities in the UC system post-settlement agreement. **C.A. Jakober**, D.M. Decker

11:25 Concluding Remarks.

Cannabis: A Growing Sector for Business & Employment

Sponsored by SCHB, Cosponsored by CHAS

WEDNESDAY AFTERNOON

Section A

Park Central San Francisco

Olympic

What Have We Learned & Where Are We Going: Post-Settlement in the University of California

Cosponsored by CCS and PRES

D. M. Decker, J. Palmer, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 CHAS **47.** Establishing a student-enforced safety culture in academic research labs. **K.A. Miller**

2:00 CHAS **48.** Successfully implementing a positive safety culture in an R1 research laboratory as a graduate safety officer. **B. Armstrong**, A.K. Franz

‡ *Cooperative Cosponsorship*

2:25 CHAS **49.** Heavy lifting of compliance: A graduate student perspective. **A. Manlove**, **B. Anderson**, **N. Nunez**

2:50 Intermission.

3:05 CHAS **50.** UC-Davis: SOP task force committee. **P.N. Serrano**

3:30 CHAS **51.** Continuing to promote careful chemistry in the post-settlement era. **J.G. Palmer**, **L.S. Wong**

3:55 Concluding Remarks.

rience. **K. Deards**, **S. Krane**, **R. Guha**, **A. Magid**

11:40 Panel Discussion.

Computer-Aided Peptide Design

In-Silico Peptide Modeling

Sponsored by COMP, Cosponsored by CINF

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Sponsored by COMP, Cosponsored by CINF

CINF

Division of Chemical Information

E. Alvaro, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin (see *COMP,* Tue)

Applications of Cheminformatics & Computational Chemistry in Environmental Health (see *ENVR,* Wed, Thu)

SOCIAL EVENTS:

Reception, 6:30 PM: Sun

Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

Business Meetings, 12:30 PM & 3:00 PM: Sat

SUNDAY MORNING

Section A

Park Central San Francisco

Metropolitan I

Materials Informatics & Computational Modeling

Cosponsored by COMP and POLY

R. J. Bienstock, M. A. Pasquinelli, *Organizers*, *Presiding*

8:30 CINF **1.** Computer-aided design of novel materials with desired electronic and physical properties. T. Moot, **O. Isayev**, J. Cahoon, A. Tropsha

8:55 CINF **2.** Leveraging informatics and machine learning to predict physical properties of organic compounds. **M. Liosi**, T. Spyriouni, X. Krokidis, **L. Subramanian**

9:20 CINF **3.** Rational materials design *via* machine learning. **J. Hachmann**

9:45 Intermission.

9:50 CINF **4.** Machine learning for large-scale MOF screening. **D. Coupry**, L. Groot, M.A. Addicoat, T. Heine

10:15 CINF **5.** Accelerating materials research through the effective use of data. **T. Mueller**

10:40 CINF **6.** Dark reactions project: Machine learning-assisted materials discovery using failed experiments. **J. Schrier**

11:05 Intermission.

11:10 CINF **7.** Predicting properties of organic materials with models that blend informatics with quantum chemistry. **D. Yaron**, H. Li, C.R. Collins

11:35 CINF **8.** Computer-based design of advanced materials: Chemically specific multiscale modelling of polymer-clay nanocomposites. **P.V. Coveney**, J. Suter, D. Groen

Section B

Park Central San Francisco

Metropolitan II

Open Access: Current Landscape, Challenges & Future Directions

E. Kajosalo, Y. Li, *Organizers*

G. Baysinger, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CINF **9.** Perspectives on open access. **M.G. Hicks**

9:05 CINF **10.** Current landscape and the future direction of open access publishing. **J. Heber**

9:35 CINF **11.** Setting a fee for publication. **J. McLennan**

10:05 Intermission.

10:20 CINF **12.** Free the science: Innovations and business model for scientific publishing. **M. Yess**

10:50 CINF **13.** Open access and the Royal Society of Chemistry. **R. Kidd**, R. Anand

11:20 CINF **14.** American Chemical Society's view of open access. **D.P. Henderson**

11:50 Concluding Remarks.

Section C

Park Central San Francisco

Metropolitan III

Careers in Chemical Information

S. K. Cardinal, K. Deards, *Organizers*

K. Deards, *Presiding*

8:10 Introductory Remarks.

8:15 CINF **15.** Twenty five years in cheminformatics: A career path through a diverse series of roles and responsibilities. **A.J. Williams**

8:45 CINF **16.** Old chemists never die; They just go through transformations. **D. Alberts**

9:05 CINF **17.** Challenges of the corporate librarian vs. academic librarian. **V.K. Tucci**

9:25 CINF **18.** Computational chemistry career at the NIH. **R.J. Bienstock**

9:45 Intermission.

10:00 CINF **19.** Interpreting chemistry: A day in the life of a data curator. **S. Ward**, M.P. Lightfoot, A. Sarjeant

10:20 CINF **20.** Do's and don'ts of the job search: What you need to know to succeed. **K. Deards**

10:40 CINF **21.** Preparing for careers in chemical information: A diversity of experience. **K. Deards**, **S. Krane**, **R. Guha**, **A. Magid**

11:40 Panel Discussion.

Computer-Aided Peptide Design

In-Silico Peptide Modeling

Sponsored by COMP, Cosponsored by CINF

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Sponsored by COMP, Cosponsored by CINF

SUNDAY AFTERNOON

Section A

Park Central San Francisco

Metropolitan I

Materials Informatics & Computational Modeling

Cosponsored by COMP and POLY

R. J. Bienstock, M. A. Pasquinelli, *Organizers*, *Presiding*

1:30 CINF **22.** Computational studies of interfacial fracture in polymer composite materials. **R.M. Elder**, M.S. Walter, D. Knorr, T.W. Sirk

1:55 CINF **23.** Guiding the synthesis of polyester electrolytes with hydrophobicity calculations. **R.T. Mathers**

2:20 Intermission.

2:25 CINF **24.** Challenges and opportunities in modeling UV-Vis absorption spectra of organic chromophores: Utilization of Max A. Weaver Dye Library for TD-DFT benchmarking. **E. Jakubikova**

2:50 CINF **25.** Design and optimization of polymers with high charability and high Tg using machine learning. R. Chaudret, **L. Subramanian**, R. Avakian, A. Mukhopadhyay

3:15 Intermission.

3:20 CINF **26.** Quasi one-dimensional transport mechanisms in superionic conductors. **J. Eapen**, A. Annamareddy

3:45 CINF **27.** Prediction of salt-responsive morphological phase diagrams for polyelectrolytes in semidilute regime. N.K. Li, T.A. Deaton, **Y.G. Yingling**

4:10 CINF **28.** Thermal conductivity and reduced-order approximation based on covariance of heat current. **J. Eapen**, A. Raj

Section B

Park Central San Francisco

Metropolitan II

Open Access: Current Landscape, Challenges & Future Directions

G. Baysinger, Y. Li, *Organizers*

E. Kajosalo, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 CINF **29.** Open access activities at Thieme publishers. **S. Haak**

1:50 CINF **30.** Open research at Springer Nature. **N. Quaderi**

2:20 CINF **31.** Seeing the forest for the trees: What's happening around the world with open access? **A. Wise**, P. Carton

2:50 CINF **32.** Open access to chemical information. **J. Zhang**, P.A. Thiessen, A. Gindulyte, E. Bolton

3:20 Intermission.

3:35 CINF **33.** ArXiv and SCOAP3: Evolution of open access and funding models. **C. Hoover**

4:05 CINF **34.** bioRxiv: The development of a preprint service for the life sciences. **J.R. Inglis**

4:35 CINF **35.** ChemRxiv – Building a preprint server for the benefit of the chemistry community. K. Davies, **D.P. Henderson**

5:05 Concluding Remarks.

Section C

Park Central San Francisco

Metropolitan III

Textbooks & the Practice of Science: Before, During & After Gutenberg

Cosponsored by CHED and HIST‡

R. E. Belford, T. Gupta, *Organizers*

G. D. Patterson, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CINF **36.** William Henry and The Elements of Experimental Chemistry. **G.D. Patterson**

1:55 CINF **37.** Cannizzaro's sunto: A legendary text of chemistry. **C.J. Giunta**

2:15 CINF **38.** Alexandre Édouard Baudrimont and his Introduction à l'étude de la chimie par la théorie atomique (Introduction to the Study of Chemistry by the Atomic Theory). **V.V. Mainz**

2:35 CINF **39.** Chemistry for a popular audience: Josiah Parsons Cooke's The New Chemistry. **R.A. Egolf**

2:55 Intermission.

3:10 CINF **40.** Basic organic textbook: From its beginning to its (digital) end. **M.C. Caserio**

3:30 CINF **41.** Mechanistic turn in inorganic textbooks: Basolo and Pearson's Mechanisms of Inorganic Reactions. **J.A. Labinger**

3:50 CINF **42.** Edgar Fahs Smith and elements of chemistry at Penn. **G.D. Patterson**

4:10 CINF **43.** Panel discussion on lessons learned from historical textbooks. **G.D. Patterson**

4:30 Concluding Remarks.

Computer-Aided Peptide Design

Computational Approaches to Peptide ADME

Sponsored by COMP, Cosponsored by CINF

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Sponsored by COMP, Cosponsored by CINF

SUNDAY EVENING

Section A

Park Central San Francisco

Franciscan I & II

CINF Scholarships for Scientific Excellence: Student Poster Competition

S. J. Chalk, *Organizer*

6:30 - 8:30

CINF **44.** Application of spectral and diffusion geometry descriptors to shape-based virtual screening. **M. Seddon**, D. Cosgrove, M. Packer, V.J. Gillet

CINF **45.** Evaluating performance of chemical fingerprinting methods and machine learning algorithms for in silico prediction of Ames mutagenicity. **D. Mehta**, P. Volarath, K. Arvidson

CINF **46.** Shape described by numbers – Comparing the shape fingerprint and shape multipole methods. **J. Zarnecka**, A.G. Leach, S.J. Enoch

CINF **47.** Water, water, everywhere...: Modeling water molecules in protein-ligand complexes. **E. Nittinger**, P.A. Gibbons, V. Tsui, D.F. Ortwine, M. Rarey

CINF **48.** Mobilizing EPA's Comptox Chemistry Dashboard data on mobile devices. K. Blinov, **A. McEachran**, A.J. Williams

CINF **49.** Free online access to experimental and predicted chemical properties through the EPA's CompTox Chemistry Dashboard. **K. Mansouri**, C. Grulke, R. Judson, A.J. Williams

CINF **50.** Cheminformatics modeling of closantel analogues potentially relevant for creating river blindness. **M.A. Kuenemann**, S. Kuchibhotla, P. Kyaw Zin, D. Fourches

CINF **51.** Generation of structure-based pharmacophores in unbound state (apo) protein binding sites. **T. Seidel**, V. Reiner, G. Ibis, T. Langer

CINF **52.** Visualization in CDD vault: A new reactive web platform for multidimensional drug discovery data mining and visualization. **W.W. Smith**, B.A. Bunin, K. Gregory

CINF **53.** Investigating transport properties with multi-scale computable mesh models from heterogeneous structural datasets. **C. Lee**, J. Moody, J. McCammon, M. Holst, R.E. Amaro

CINF **54.** Toward automated verification of curated chemical property data. **A. Loyola**, S.J. Chalk

CINF **55.** Withdrawn.

CINF **56.** Semantically capturing NIST SRD 81 data using the SciData data model. **T. Schumann**, S.J. Chalk

MONDAY MORNING

Section A

Park Central San Francisco

Metropolitan I

Advances in High-Throughput Screening

Cosponsored by COMP and MEDI

R. J. Bienstock, S. Sirimulla, *Organizers*, *Presiding*

8:15 Introductory Remarks.

8:20 CINF **57.** Maximizing PubChem for drug discovery. **S. Kim**, E. Bolton, S.H. Bryant

8:45 CINF **58.** Web servers and high throughput virtual screening. **R.J. Bienstock**

9:10 CINF **59.** Recent advances in Autodock Vina molecular docking software. **S. Sirimulla**

9:35 Intermission.

9:45 CINF **60.** Hyperspace, warp speed and time warp: Searching the chemical universe at ludicrous speed. **C. Detering**

10:10 CINF **61.** PubChem BioAssay: What it takes to build a public HTS data warehouse. **Y. Wang**

10:35 CINF **62.** Confidently targeting high quality hits from high-throughput screening. **M.D. Segall**, T. Mansley, P. Hunt, E. Champness

11:00 Intermission.

11:10 CINF **63.** Discovery of novel inhibitors of the galactokinase from high throughput and *in silico* screening. **M. Shen**, X. Hu, Y. Zhang, L. Liu, M. Boxer, M.D. Hall

11:35 CINF **64.** Structural modeling and identification of small molecule agonists of human relaxin family peptide receptor 1. **X. Hu**, C. Myhr, E. Barnaeva, I. Agoulnik, M. Ferrer, J.J. Marugan, N. Southall, A. Agoulnik

Section B

Park Central San Francisco

Metropolitan II

Advances in Data Visualization

E. Davis, *Organizer, Presiding*

8:10 Introductory Remarks.

8:15 CINF **65.** Expanding the target dimension: How to visualize a lot of models. **A. Clark**

8:40 CINF **66.** Visualizing molecules in and out of context. C. Batchelor, N. Bailey, P. Corbett, **J. White**, J. Boyle

9:05 CINF **67.** Withdrawn.

9:30 CINF **68.** Scaffold histories: Visualizing temporal trends in scaffold properties. **B. Zdrazil**, R. Guha

9:55 Intermission.

10:10 CINF **69.** Shoring up the (data) base: Advances in materials data processing and visualization. **P. Schaal**, R. Padilla, S.J. Chalk, M. Klinge

10:35 CINF **70.** Data visualisation: Saying it all in a bite-sized chunk. **E. Champness**, M.D. Segall, P. Hunt, T. Mansley

11:00 CINF **71.** Scalable web-based molecular graphics and visualization of structure quality metrics. **A.S. Rose**, A.R. Bradley, Y. Valasatava, J. Duarte, A. Prlic, P. Rose

11:25 CINF **72.** Semi-interactive creation of 2D protein-ligand pose diagrams with PoseView-2. T. Otto, **M. Rarey**

11:50 Concluding Remarks.

Section C

Park Central San Francisco

Metropolitan III

Textbooks & the Practice of Science: Before, During & After Gutenberg

Cosponsored by CHED and HIST‡

R. E. Belford, G. D. Patterson, *Organizers*

T. Gupta, *Organizer, Presiding*

8:45 Introductory Remarks.

8:50 CINF **73.** Extensible electronic textbook. **R.E. Belford**, J.L. Holmes

9:10 CINF **74.** Supporting transmission of knowledge for chemical safety education: An information workflow supplement to the laboratory textbook. **L. McEwen**, S.B. Sigmann, R. Stuart

9:30 CINF **75.** Chemistry in context: How do we most effectively engage the non-science majors? **B.D. Fahlman**

9:50 CINF **76.** Facts versus foundation -- The evolution of learning needs for contemporary science students. **A.S. Tseng**

10:10 Intermission.

10:25 CINF **77.** Indian textbooks: From the beginnings to the modern times. **P. Roy Chowdhury**

10:45 CINF **78.** Alchemy to chemical science: The advance of texts for over 5,000 years in China from the oracle bones to e-learning resources and methodologies. **R.J. Rusay**, B. Koo, R. Daugherty, G. Dasgupta, D.S. Larsen

11:05 CINF **79.** Instructor support is key to adoption of open educational systems. **J.B. Halpern**, D.S. Larsen

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Sponsored by COMP, Cosponsored by CINF

MONDAY AFTERNOON

Section A

Park Central San Francisco

Metropolitan I

Advances in High-Throughput Screening

Cosponsored by COMP and MEDI

R. J. Bienstock, S. Sirimulla, *Organizers*, *Presiding*

1:15 Introductory Remarks.

1:20 CINF **80.** Spectral and diffusion geometry descriptions of molecular shape. **M. Seddon**, D. Cosgrove, M. Packer, V.J. Gillet

1:45 CINF **81.** Rapid, accurate, precise and reliable relative free energy prediction using ensemble based thermodynamic integration. A.P. Bhati, S. Wan, D.W. Wright, **P.V. Coveney**

2:10 CINF **82.** Advanced HTS triage methods to identify false negative compounds. **L. Zhang**, M. Boehm, F.E. Lovering

2:35 Intermission.

2:45 CINF **83.** Withdrawn.

3:10 CINF **84.** Combining *de novo* design and macromolecular target prediction for high-throughput virtual screening. **G. Schneider**, L. Friedrich, A. Button, P. Schneider

3:35 CINF **85.** Chemical biology informatic approaches to enable high-throughput screening: Focused compounds sets, target enrichment, and hit expansion. **P. Kutchukian**, A. Wassermann, I. Wallace, C. Chang, W.L. Petrilli, T. Kreamer, M. Kansara, C.L. Waller, J.E. Imbriglio, M. Glick

4:00 Intermission.

4:10 CINF **86.** AbbVie target prediction tool. **A. Seal**, **R. Gupta**, D. Debe, P. Hajduk

4:35 CINF **87.** Open innovation drug discovery: Structure blinded virtual screening. **N.I. Franklin**

5:00 Concluding Remarks.

Section B

Park Central San Francisco

Metropolitan II

The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit

Cosponsored by CHED, CPRM and ETHX‡

J. N. Currano, P. A. Mabrouk, *Organizers*, *Presiding*

1:10 Introductory Remarks.

1:15 CINF **88.** Authorship issues in academia of low and lower middle-income countries. **L. Anestidou**

1:40 CINF **89.** What constitutes authorship? Guidance from the Committee on Publication Ethics (COPE). **H.L. Tierney**

2:05 CINF **90.** Teaching students where credit is due: Attribution 101 for the mash-up generation. **J.N. Currano**

2:30 CINF **91.** Influence of graduate students on authorship decision-making in undergraduate research partnerships. **A. Andes**, P.A. Mabrouk, A. Pattani

2:55 Intermission.

3:10 CINF **92.** Authorship issues and conflict in the U.S. academic chemical community. **J. Seeman**

‡ *Cooperative Cosponsorship*

3:35 CINF **93.** ORCID iDs & Project Credit: Contributor badges and getting credit for your work. **C. Craig**

4:00 CINF **94.** Do not lose your invention by improperly naming inventors on the patent. **X. Pillai**

4:25 CINF **95.** Hey—You stole my invention! Avoiding ethical pitfalls in determining inventorship, authorship, and honoring Non-Disclosure Agreement (NDA) obligations. **J.L. Krieger**

4:50 Discussion.

5:05 Concluding Remarks.

Section C

Park Central San Francisco

Metropolitan III

Textbooks & the Practice of Science: Before, During & After Gutenberg

Cosponsored by CHED and HIST‡

T. Gupta, G. D. Patterson, *Organizers*

R. E. Belford, *Organizer, Presiding*

1:50 Introductory Remarks.

1:55 CINF **96.** Developing and assessing effective cyberlearning within the Libretexts libraries. **D.S. Larsen**

2:15 CINF **97.** Textbooks in transition: A new low-cost model for distributing chemistry textbooks and tools. **M.A. Bishop**

2:35 CINF **98.** Democratization of learning and re-embedding the textbook. **B. McCollum**

2:55 CINF **99.** MindTap general chemistry: Integrating scientific exploration and problem-solving within a textbook. **W.J. Vining**, S.M. Young, R. Day

3:15 Intermission.

3:30 CINF **100.** What should a textbook for 21st-century students look like? **J. Moore**, C.L. Stanitski

3:50 CINF **101.** High school students and critical reading of science misinformation and inaccurate claims. **A.S. Tseng**

4:10 CINF **102.** Textbooks and the SI base units. A challenge for authors and editors. **P.F. Rusch**

4:30 CINF **103.** Panel discussion on textbooks of the future. **R.E. Belford**

4:50 Concluding Remarks.

Data Science Challenges in Computational Chemistry

Sponsored by COMP, Cosponsored by CINF

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Sponsored by COMP, Cosponsored by CINF

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

E. Alvaro, *Organizer*

8:00 - 10:00

28, 44-45, 48-51, 53-54, 56, 86-87, 91, 101. See previous listings.

108, 121, 139, 160. See subsequent listings.

TUESDAY MORNING

Section A

Park Central San Francisco

Metropolitan I

Text-Mining & Natural Language Processing for Chemical Information: From Documents to Knowledge

R. J. Bienstock, J. L. Nauss, *Organizers*, *Presiding*

9:00 CINF **104.** From documents to knowledge. **J.L. Nauss**

9:25 CINF **105.** Improving chemical names matching for verification, rating, and validation of PubChem compound records. **L. Zaslavsky**, D.M. Lowe, C. Wei, Z. Lu, E. Bolton

9:50 CINF **106.** Advanced grammars for state-of-the-art Named Entity Recognition (NER). **R.A. Sayle**, D.M. Lowe

10:15 Intermission.

10:30 CINF **107.** Mining protein interactions from biomedical literature using semantic similarity. C. Schmitt, S. Cox, L. Christopherson, E. Scott, S. Firrincieli, N. Baker, E. Tutubalina, **A. Tropsha**

10:55 CINF **108.** Automatic extraction of bioactivity data from patents. **D.M. Lowe**, S. Senger, R.A. Sayle

11:20 CINF **109.** Text-mining strategies to support computational research in chemical toxicity. **N. Baker**, T. Knudsen, A.J. Williams, K. Crofton

Section B

Park Central San Francisco

Metropolitan II

Open Access: Current Landscape, Challenges & Future Directions

G. Baysinger, E. Kajosalo, *Organizers*

Y. Li, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CINF **110.** Increasing public access to federally-funded R&D results – The Department of Energy's Access Model and DOE PAGES. **B. Hitson**, J. Gilmore, C. Robinson, S. Studwell

9:05 CINF **111.** Building communities and infrastructure to support openness. **S. Bowman**

9:35 CINF **112.** Open access reporting: Improving the accuracy of data collection during the publishing process. **M. Qiu**, S. Akay, M. Blickem, S. Monasky

10:05 Intermission.

10:20 CINF **113.** Getting more than what you're paid for: Technologies driving revenue in an OA landscape. **J. Wilcock**

10:50 CINF **114.** CHORUS – Driving the uptake and monitoring of public access by leveraging established standards and infrastructure for cost efficiency. **S. King**

11:20 CINF **115.** Tales from the front lines: Supporting open access journals & repositories with research metrics. **A. Michalek**

11:50 Concluding Remarks.

Section C

Park Central San Francisco

Metropolitan III

Advanced Materials: Issues in Nanoinformatics & Nanosafety Data

Y. Cohen, M. G. Hicks, R. Liu, L. McEwen, *Organizers*, *Presiding*

8:10 Introductory Remarks.

8:15 CINF **116.** Meeting the challenges of nanoinformatics. **J. Rumble**

8:40 CINF **117.** Conceptual analysis and chemical information: A case study in nanoscience. **J.R. Bursten**

9:05 CINF **118.** Nanoinformatics platform for environmental impact assessment of engineered nanomaterials. **M. Bilal**, **P. Church**, H. Liu, R. Liu, Y. Cohen

9:30 CINF **119.** Materials informatics: Computational and cheminformatics approaches towards properties assessment and rational design of advanced materials. **B. Rasulev**

9:50 Intermission.

10:05 CINF **120.** QNAR models for the rational design of nanomaterials. **D. Fourches**

10:30 CINF **121.** Data visualization tool for exploring how nanomaterial properties correlate with toxicity in zebrafish assays. **G. Lowry**, S. Karcher, C. Hendren, M. Wiesner, B. Harper, S. Harper

10:55 CINF **122.** Investigation of the interactions of macrophage and silver nanowires. **E. Ogorodnik**, **G. Liu**

11:20 CINF **123.** Flexible database management system for nanoinformatics research and data integration. **P. Church**, M. Bilal, R. Liu, Y. Cohen

11:45 CINF **124.** Tools and approaches for data deposition into nanomaterial databases. **V. Tkachenko**, R. Zakharov, A. Kabanov, K. Mills, T. Hickey, A. Tropsha

Information Flow in Environmental Health & Safety

Sponsored by CHAS, Cosponsored by CCS and CINF‡

TUESDAY AFTERNOON

Section A

Park Central San Francisco

Metropolitan I

Text-Mining & Natural Language Processing for Chemical Information: From Documents to Knowledge

R. J. Bienstock, J. L. Nauss, *Organizers*, *Presiding*

2:00 CINF **125.** Making the old new again: Modern technology provides access to historical chemical information. **S.P. Kuhn**, J. Tinsley, K.C. Schwall

2:25 CINF **126.** Evolution of SciFinder to meet the changing needs for scientific information. **P.Y. Ayala**, Y. Wu, G. Gao, J.W. Taylor

2:50 CINF **127.** Trends and relations. P. Corbett, N. Bailey, C. Batchelor, **J. White**, J. Boyle

3:15 Intermission.

3:30 CINF **128.** ChemAnalyzer: A text analytics platform for chemical surveillance. **S. Gaurav**, **T. Roy**, **J. Zeng**, **L. E Charles**, **M. Henry**, **K. Han**, **C. Corley**

3:55 CINF **129.** Addition of chemical search capabilities to PATENTSCOPE: Turning a full-text search system into a chemistry database. **J. Eiblmaier**, C. Mazenc, D. Geppert, L. Isenko, H. Saller

4:20 CINF **130.** ChemExtractor: Enhanced rule-based capture and identification of PDF based property data. **S.J. Chalk**, T. Schumann, A. Loyola, M. Bastien, J. Turner

Section B

Park Central San Francisco

Metropolitan II

Open Access: Current Landscape, Challenges & Future Directions

G. Baysinger, Y. Li, *Organizers*

E. Kajosalo, *Organizer, Presiding*

1:15 Introductory Remarks.

1:20 CINF **131.** Open up the open access conversation at a STEM-focused university. **Y. Li**

1:50 CINF **132.** Work in progress: Status of open access at a major research university. **G. Baysinger**

2:20 CINF **133.** Qualitative analysis of the Berkeley Research Impact Initiative (BRII) open access fund at UC Berkeley. **S. Teplitzky**

2:50 CINF **134.** Open software in chemistry: Challenges and opportunities. **L. Soito**

3:20 Intermission.

3:35 CINF **135.** Using Caltech's institutional repository to track OA publishing in chemistry. **D. Wrublewski**, G.S. Porter

4:05 CINF **136.** Impact of recent changes at MIT Libraries on MIT open access policy. **E. Kajosalo**

4:35 CINF **137.** What price open access: Findings from the Pay It Forward Project. **I. Anderson**

5:05 Concluding Remarks.

Information Flow in Environmental Health & Safety

Sponsored by CHAS, Cosponsored by CCS and CINF‡

WEDNESDAY MORNING

Section A

Park Central San Francisco

Metropolitan I

Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

Cosponsored by COMP

R. J. Bienstock, B. A. Bunin, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:40 CINF **138.** CCDC: A public-private research partnership. **P. Davie**, I. Bruno

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

9:05 CINF **139.** PubChem BioAssay: Grow with the support of the community. **Y. Wang**

9:30 CINF **140.** Selection of cross-docking candidates and comparison of evaluation metrics in Continuous Evaluation of Ligand Pose Prediction (CELPP). **S. Liu**, J. Wagner, C. Churas, S.M. Gathiaka, J. Grethe, M. Chiu, H. Yang, S. Burley, R.E. Amaro, M.K. Gilson

9:55 Intermission.

10:05 CINF **141.** Synthetically accessible virtual inventory (SAVI). Y. Pevzner, W. Ihlenfeldt, **M.C. Nicklaus**

10:30 CINF **142.** Cross-platform HELM editor empowers HELM adoption. **J. Lee**, R. Hotchandani

10:55 CINF **143.** HELM: A line-notation and software infrastructure for managing biopolymers. **J. Milton**

11:20 CINF **144.** Tangled up in data: Enabling strong collaborations with transparent information sharing. **J. Neitz**

Section B

Park Central San Francisco

Metropolitan II

General Papers

E. Alvaro, *Organizer, Presiding*

8:15 Introductory Remarks.

8:20 CINF **145.** Withdrawn.

8:40 CINF **146.** PubChem's literature and patent information for drug discovery. **S. Kim**, P.A. Thiessen, T. Cheng, B. Yu, B.A. Shoemaker, J. Wang, E. Bolton, Y. Wang, S.H. Bryant

9:00 CINF **147.** QUDT toolkit: Development of framework to allow management of digital scientific units. **S.J. Chalk**, R. Hodgson, S. Ray

9:20 CINF **148.** Mapping the 3D structures of small molecule binding sites. **J. Meyers,** N. Brown, J. Blagg

9:40 CINF **149.** Predictions are tough, especially about the future: Assessing model quality, need for rapid automated model updates, and distributed computing. **V.R. Polyakov**, E.J. Martin

10:00 Intermission.

10:15 CINF **150.** HLA-triggered adverse drug reactions: Challenges and opportunities for molecular modeling. **G. Van Den Driessche**, D. Fourches

10:35 CINF **151.** Can machine learning methods usefully rank small molecules for their selective growth inhibition of cancer cell lines with the BRAF V600E gene mutation? **J. Langham**

10:55 CINF **152.** Using the Structured Product Labeling format to index versatile chemical data. **V. Tkachenko**, Y. Borodina, A.J. Williams

11:15 CINF **153.** Reinventing the IUPAC Gold Book. **S.J. Chalk**, M. Kinnan, L. McEwen, H.A. Lawlor, D. Martinsen

11:35 CINF **154.** Computational screening of hydrogen storage in experimental metal-organic frameworks. **Y. Chung**

Section C

Park Central San Francisco

Metropolitan III

Assessment of Chemistry Collections & Services

V. F. Scalfani, A. B. Twiss-Brooks, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CINF **155.** What about the books? Usage trends of chemistry monographs among graduate students in an era of transition. **D.W. Flaxbart**

9:00 CINF **156.** Matching chemistry collections and user needs: A data-driven approach. **E. Alvaro**

9:25 CINF **157.** Assessment of chemistry thesis and dissertation titles for collection development. **V.F. Scalfani**

9:50 Intermission.

10:05 CINF **158.** Chemistry library as rallying point: Assessing how to save a branch library. **J.R. Garritano**

10:30 CINF **159.** Withdrawn.

10:55 CINF **160.** Assessing data management practices and needs through data management plans. **B. Westra**

11:20 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Park Central San Francisco

Metropolitan I

Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

Cosponsored by COMP

R. J. Bienstock, B. A. Bunin, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 CINF **161.** Extracting medicinal chemistry knowledge by a secure matched molecular pair analysis platform: Standardization enables merging with public data. **A. Dossetter**, E.J. Griffen, A.G. Leach, S. Montague

2:00 CINF **162.** Enabling precision drug repurposing through innovative public-private partnerships. **D.J. Wild**, J.J. Yang

2:25 CINF **163.** Innovative medicines initiative: From semantic data integration to risk assessment. D. Digles, D. Goldmann, B. Zdrazil, **G.F. Ecker**

2:50 Intermission.

3:00 CINF **164.** Present and futuristic collaborative drug discovery informatics innovations (CDD vault + bioassay express). **B.A. Bunin**

3:25 CINF **165.** Supporting compound optimisation in not-for-profit and academic research. **M.D. Segall**, T. Mansley, P. Hunt, K. Chibale, T. Paquet, J. Duffy

3:50 CINF **166.** tranSMART platform for translational medicine: An open source, open data and open science platform. **R. Potenzone**, K. Elliston

4:15 Discussion.

4:30 Concluding Remarks.

Section B

Park Central San Francisco

Metropolitan II

General Papers

E. Alvaro, *Organizer, Presiding*

1:00 CINF **167.** VIMAL: A chemoinformatics toolkit for design of novel antiviral agents through textmining of scientific literature. M. Karthikeyan, **R. Pahujani**, R. Vyas

1:20 CINF **168.** Know the breadth of your sources: The CAS content collection is your comprehensive resource. **E.N. Cheeseman**

1:40 CINF **169.** Streamlining pharmaceutical supply chain processes: The emerging application of solid-state structural informatics. **M.J. Bryant**, A.G. Maloney, N. Feeder

2:00 CINF **170.** Open Science Data Repository - the platform for materials research. **V. Tkachenko**, R. Zakharov, I. Presniakov, S. Kalmykov

2:20 CINF **171.** Software tool that provides the critical information needed to enable toxicity-focused research. **N. Vaidya**

2:40 Intermission.

2:55 CINF **172.** Chemistry Validation and Standardization Platform Version 2.0. **V. Tkachenko**, R. Zakharov, C. Grulke, A.J. Williams

3:15 CINF **173.** Withdrawn.

3:35 CINF **174.** ZINC: A free database of commercially available compounds for virtual screening. **J.J. Irwin**

3:55 CINF **175.** Biomedical literature mining for protein-protein interactions analysis using electronic mailing system. **M. Karthikeyan**, **R. Vyas**

CHAL

Division of Chemistry and the Law

K. Bianco and J. Kennedy, *Program Chairs*

SOCIAL EVENTS:

Luncheon, 12:00 PM: Mon

Reception, 6:00 PM: Mon

BUSINESS MEETINGS:

Business Meeting, 5:00 PM: Sun

SUNDAY AFTERNOON

Section A

Park Central San Francisco

Stanford

Strengthening Your Patent Rights in Light of Recent Federal Circuit Court Decisions

A. H. Berks, *Organizer*

X. Pillai, *Organizer, Presiding*

A. Berks, *Presiding*

1:00 CHAL **1.** Review of recent Federal Circuit decisions relevant to what scientists need to know about patent filing and prosecution. **X. Pillai**, **A. Berks**

MONDAY MORNING

Section A

Park Central San Francisco

Stanford

Non-Traditional Careers in Chemistry

K. E. Bianco, *Organizer*

R. Franz, *Presiding*

9:00 CHAL **2.** Alternative careers in chemistry, an international perspective. **R. Franz**

9:30 CHAL **3.** A PhD is not enough—Working at the intersection of science and business. **J. Chen**

Section B

Park Central San Francisco

Stanford

Patent Challenges & Chocolate: A Sweet & Sour Symposium

J. J. Hasford, *Organizer, Presiding*

10:30 CHAL **4.** Interplay between patent office IPR challenges and district court patent infringement cases. **J.J. Hasford**

11:00 CHAL **5.** Chocolate: Food of the Gods - 2016 Helen Free Award Lecture. **H.M. Peters**, **S.B. Peters**

Chemical Forensics

Investigations of Alleged Use & Source Attribution of Chemical Weapons

Sponsored by ANYL, Cosponsored by CHAL and PRES

MONDAY AFTERNOON

Section A

Park Central San Francisco

Stanford

The Use of Scientific Information in IP-Related Matters

E. N. Cheeseman, *Organizer, Presiding*

1:30 CHAL **6.** What exactly are you looking for? Searching for chemical information. **E.N. Cheeseman**

2:00 CHAL **7.** Patent claims reciting scientific information: The now heightened definiteness requirement. **T.A. Ostomel**

2:30 CHAL **8.** Your next breakthrough starts here – CAS content and solutions foster discovery and innovation. **K. Zielenbach**

3:00 CHAL **9.** Survey of biosequence in patent claims and the impact on biosequence search methods. **K.L. Hoppe**

3:30 CHAL **10.** Patents and basic scientific research: Discovery versus invention. **P. Campbell**

4:00 CHAL **11.** Importance of Markush searching for FTO purposes. **P.F. Blasi**

Chemical Forensics

Chemical Attribution Signatures of Illicit Drugs & Toxic Chemicals

Sponsored by ANYL, Cosponsored by CHAL and PRES

‡ *Cooperative Cosponsorship*

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

K. E. Bianco, J. L. Kennedy, *Organizers*

8:00 - 10:00

CHAL **12.** Chocolate: Food of the gods. **H.M. Peters**, **S.B. Peters**

CHAL **13.** National Inventors Hall of Fame 2017. **H.M. Peters**, **S.B. Peters**

TUESDAY MORNING

Section A

Park Central San Francisco
Stanford

An International Perspective: Patent Eligible Subject Matter & Opposition Procedures

K. E. Bianco, *Organizer*

J. Gledhill, *Organizer, Presiding*

9:00 CHAL **14.** Patent opposition and invalidation procedures: What is the same and what differs in Australia, Europe, the United States, and China? **K.E. Bianco**, **L. Wall**, **J. Gledhill**, **S. Zou**

10:00 CHAL **15.** Hot topics in international patent law: What is allowable patent eligible subject matter? **K.E. Bianco**, **J. Gledhill**, **L. Wall**, **S. Zou**

11:00 CHAL **16.** Silicon Valley Regional Office of the U.S. Patent and Trademark Office. **J. Cabeca**

Chemical Forensics

Chemometrics & Statistics for Signature Discovery & Exploitation

Sponsored by ANYL, Cosponsored by CHAL and PRES

TUESDAY AFTERNOON

Section A

Park Central San Francisco
Stanford

Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce

Cosponsored by CHAS, ENVR and I&EC

I. Hantman, *Organizer, Presiding*

2:30 CHAL **17.** Recent developments in TSCA regulation: New requirements for chemicals in commerce. **I. Hantman**, **D.K. Liu**, **K. Matthews**, **M. Doa**

Section B

Park Central San Francisco
Stanford

Protecting & Capitalizing on Your Intellectual Property

J. L. Kennedy, *Organizer, Presiding*

12:00 CHAL **18.** Chemical patents: How to navigate the changing legal landscape to protect your chemical technology. **J.L. Kennedy**

12:30 CHAL **19.** Creating an intellectual property strategy and portfolio. **J.L. Kennedy**, J. Link

1:00 CHAL **20.** Licensing: Capitalizing on patents, trade secrets, and other intellectual property. **J. Link**

Chemical Forensics

Isotopic & Elemental Profiling for the Source Attribution of Materials

Sponsored by ANYL, Cosponsored by CHAL and PRES

WEDNESDAY MORNING

Section A

Park Central San Francisco
Stanford

Cannabis Law: Navigating Complex Regulatory & Legal Issues in States with Legal Cannabis Programs

J. Marcu, *Organizer, Presiding*

9:00 CHAL **21.** Clinical and analytical confirmation of new psychoactive substances. **S. Vucinic**

9:30 CHAL **22.** Navigating complex issues in states with legal cannabis programs. **R. Mirkarimi**

10:00 CHAL **23.** Using GxP management software in conjunction with quality assurance data to maintain regulatory compliance and support process improvement in the cannabis industry. **J. Applen**

10:30 CHAL **24.** Patient Focused Certification (PFC) – Quality standards of cannabis products for medical use. **J. Marcu**, S. Sherer, P. Kubu

11:00 CHAL **25.** Intellectual property issues (and solutions) for cannabis companies. **R. Micheletti**

WEDNESDAY AFTERNOON

Section A

Park Central San Francisco
Stanford

A Decade of U.S. Supreme Court Patent Jurisprudence

R. G. Bone, *Organizer, Presiding*

2:45 CHAL **26.** Survey of a decade of U.S. Supreme Court patent cases. **R.G. Bone**

3:15 CHAL **27.** Highlights of the last decade of Supreme Court patent jurisprudence. **R.G. Bone**

Section B

Park Central San Francisco
Stanford

The Many Faces of CHAL: Where Chemistry Meets the Law

J. L. Kennedy, *Organizer*

K. E. Bianco, *Organizer, Presiding*

1:00 CHAL **28.** What is substantially similar? Interpreting federal law governing unscheduled drug-like chemicals that are substantially similar to listed controlled substances. **G.B. Dudley**

1:30 CHAL **29.** Impact of national printing inks ordinance on food packaging materials and packaged foods: New national rules during the time at harmonization of the EU rules. **K. Salmen**

2:00 CHAL **30.** Pharmaceutical products and compendial standards. **S. Ramakrishna**, **L.M. Santos**, **R.A. Femia**

COLL

Division of Colloid and Surface Chemistry

R. Nagarajan, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend (see *CATL,* Sun, Mon)

Chemical Principles of Environmental, Cellular & Organismal Nanotoxicology (see *ENVR,* Wed)

Deposition & Etching of Nanostructures (see *INOR,* Wed)

Janus Particles: Synthesis, Characterization & Applications (see *PMSE,* Sun, Mon)

Molecular Engineering of Peptide Assembly (see *PMSE,* Mon, Tue, Wed)

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts (see *PHYS,* Wed, Thu)

SOCIAL EVENTS:

Social Hour with Poster Session, 6:00 PM: Sun

Luncheon, 12:00 PM: Tue

BUSINESS MEETINGS:

COLL Program & Executive Committee Meeting, 4:00 PM: Sat

Business Meeting, 5:30 PM: Sun

SUNDAY MORNING

Section A

Moscone Center
2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

K. Morigaki, D. Y. Sasaki, *Presiding*

8:30 COLL **1.** Rationally designed peptoids insert into edge and face of bicelle structure. **H. Najafi**, S.L. Servoss

8:50 COLL **2.** Transport across droplet interface lipid bilayers via a pH gradient. **S. Dixit**, B. Guo, B. Tasseff, G.W. Faris

9:15 COLL **3.** Second harmonic generation studies of water-soluble peptoids adsorbed to phospholipid membranes. **G.Y. Stokes**, A.A. Fuller, A. Calkins, J. Rangel, M.R. Landry

9:40 COLL **4.** Lipid structure, lateral order and inter-membrane forces. **U. Raviv**, L. Fink

10:05 COLL **5.** Probing model membrane local dynamics. **T. Gutberlet**, M. Trapp, J. Peters, D. Posselt

10:30 COLL **6.** Tubulin on biomimetic mitochondrial membranes: Structural features and identification of lipid binding domain. **D.P. Hoogerheide**, S. Noskov, D. Jacobs, H. Nanda, T.K. Rostovtseva, S.M. Bezrukov

10:55 COLL **7.** Cell-free expression of biologically active integral membrane protein. **A. Vaish**, C. Chen, S. Guo

11:20 COLL **8.** Determining the mRNA nanoparticle structure using SANS and SAXS. **Y. Xia**, C.J. Bowerman, J. Chan, C. Clemente, A. Esposito, E. Miracco, B. Kangarlou, M. Nieh, E. Cheung, O. Almarsson

Section B

Moscone Center
2004

Colloidal Nanoparticle Synthesis & Assembly

Nanoparticle Synthesis

H. Htoon, Y. Sun, S. Wu, *Organizers*

H. Fan, *Organizer, Presiding*

H. Zhang, *Presiding*

8:30 COLL **9.** How is the metal precursor reduced during a synthesis of colloidal nanocrystals? **Y. Xia**

9:00 COLL **10.** Crystal phase-controlled synthesis of novel noble metal nanomaterials. **H. Zhang**

9:30 COLL **11.** Synthesis of branched and polyhedral Pd-Cu nanostructures by seed-mediated co-reduction. **M. Kunz**, S.E. Skrabalak

9:50 COLL **12.** Solvent effect on ligand-metal interactions in Pd nanoparticle synthesis. **W. Li**, S. Ivanov, S. Mozaffari, A.M. Karim

10:10 COLL **13.** Colloidal synthesis of anisotropic noble metal nanostructures. **Q. Zhang**

10:30 COLL **14.** Salt-triggered deposition of polymer-coated noble metal nanoparticles on solid surfaces. **B. De Geest**

10:50 COLL **15.** Exotic syntheses of supported metal nanoparticles via metal-in-Li solutions. **T. Xu**

11:10 COLL **16.** Seeded growth of catalytically active copper-based nanostructures. **J. Chen**

11:40 COLL **17.** Designer noble metal nanostructures: Controlled synthesis and beyond. **Y. Yin**

Section C

Moscone Center
2006

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Surface Science is Alive & Well

Cosponsored by CATL

S. H. Kim, R. M. Rioux, *Organizers*, *Presiding*

8:30 COLL **18.** Surface science meets homogeneous catalysis: Cooperative properties of electrophilic organometallic ensembles. **T.J. Marks**

9:00 COLL **19.** First-principles, microkinetic modeling, and experiments for reaction mechanisms and improved catalysts. **M. Mavrikakis**

9:30 COLL **20.** Sum frequency generation microscopy of surfaces. **S. Baldelli**

10:00 COLL **21.** Surface spectroscopy and surface microscopy of catalytic processes: From model to technological materials, from UHV to *operando* conditions. **G. Rupprechter**, C. Rameshan, K. Foettinger, Y. Suchorski

10:30 COLL **22.** Vinyl acetate formation pathways and selectivity on model metal and alloy catalyst surfaces. **W.T. Tysoe**

11:00 COLL **23.** Surface science for the 21st century. **M. Salmeron**

Section D

Moscone Center

2008

Chemistry & Physics of Tribology

Tribology Perspectives & Tribochemistry

F. Mangolini, M. Ruths, *Organizers*, *Presiding*

8:30 COLL **24.** Lowering friction while saving the world: New approaches to lubrication. **N.D. Spencer**

9:05 COLL **25.** Thermal and shear effects in boundary film formation. **W.T. Tysoe**

9:40 COLL **26.** Measuring atomic wear of graphene using local stress and heat. S. Raghuraman, M.B. Elinski, J.D. Batteas, **J. Felts**

10:00 COLL **27.** Tribochemistry of GaN, a suprisingly wear resistant semiconductor. G. Zeng, X. Yang, B.E. Koel, D. Borovac, C. Tan, N. Tansu, **B. Krick**

10:20 COLL **28.** Optimization of a ReaxFF reactive force field for modeling tribochemical reactions of Cu-S and Cu-thiol/ alkoxy systems. **J. Yeon**, W.T. Tysoe, A. Martini

10:40 COLL **29.** Tribochemical aspects of mechanical mixing in tribological contacts. **M. Dienwiebel**, P. Stoyanov, P. Romero, R. Merz, P. Stemmer, M. Moseler

11:00 COLL **30.** Effect of hydrogen and oxygen partial pressure on the tribochemistry of silicon oxide-containing hydrogenated amorphous carbon. **F. Mangolini**, K. Koshigan, M.H. Van Benthem, J. Ohlhausen, J.B. McClimon, J. Hilbert, J. Fontaine, R. Carpick

11:20 COLL **31.** Wear mechanisms and regime transitions for self-mated silicon nitride lubricated by ionic liquid/water mixtures. **A. Arcifa**, A. Rossi, N.D. Spencer

11:40 COLL **32.** Mechanochemistry at sliding interfaces – Tribopolymerization of adsorbed molecules upon mechanical shear. **S.H. Kim**

Section E

Moscone Center

2010

Coacervation: Physics, Chemistry & Biology

R. Stewart, *Organizer*

P. L. Dubin, *Organizer, Presiding*

8:30 COLL **33.** RNA-based complex coacervates. **C.D. Keating**

9:10 COLL **34.** Spanning length scales in polymeric complex coacervate self-assembly. T.K. Lytle, J. Madinya, **C.E. Sing**

9:40 COLL **35.** Sequence-encoded phase behavior of intrinsically disordered proteins. **R.V. Pappu**

10:10 COLL **36.** Asymmetric segregation of P-granules by position dependent phase separation. **F. Julicher**

10:40 COLL **37.** Intra- and intermolecular electrostatic complexes of cationic antimicrobial peptides with their anionic propeptides. N. Gomes de Oliveira Júnior, O. Franco, **R. de Vries**

11:10 COLL **38.** Intrinsic disorder and overcrowding. **V.N. Uversky**

Section F

Moscone Center

2012

Applied Biosensing Based on Functional Colloids

R. Alvarez Puebla, L. Liz Marzan, J. Sagalés, G. F. Strouse, *Organizers*

W. Parak, *Organizer, Presiding*

8:30 COLL **39.** Composite porous colloids for SERS-based biosensing. **L. Liz Marzan**

9:00 COLL **40.** Functionalizing various metallic nanostructures with highly effective multi-coordinating polymers. W. Wang, A.K. Kapur, X. Ji, **H.M. Mattoussi**

9:30 COLL **41.** Towards SERS-enabled diagnostics: Quantitative detection of glucose and other biomarkers. **A. Henry**

9:50 COLL **42.** *In-situ* SERS detection at picoliter scale using substrate-less Ag nanoparticle-based liquid marbles. **X. Ling**

10:20 COLL **43.** Low frequency vibrational mode surface enhanced Raman spectroscopy characterization of gold interactions with aqueous halides. **M. Chan**, W. Leng, P.J. Vikesland

10:40 COLL **44.** High throughput optofluidic Surface-Enhanced Raman Spectroscopy (SERS) interrogation: Proof of concept via lectin detection of cancerous cells. **M. Willner**, K. McMillan, M. Zagnoni, D. Graham, P.J. Vikesland

Section G

Moscone Center

2001

Interfacial Phenomena & the Oil-Water Interface

Financially supported by The Dow Chemical Company

C. Acevedo, C. J. Tucker, *Organizers*

C. E. Mohler, *Organizer, Presiding*

8:30 COLL **45.** Nanoengineering water-in-diesel/biodiesel microemulsion interfaces to minimise particulate and NOx emissions from diesel engines to minimise atmospheric pollution. **P.A. Sermon**

8:50 COLL **46.** *Uloborus walckenaerius* bioinspired attachable, self-standing, nanofibrous membrane for versatile use in oil–water separation. **M. Tenjimbayashi**, K. Sasaki, J. Abe, S. Shiratori

9:10 COLL **47.** Interfacial interactions of granular particles with floating crude oil under different granular flow regimes. **D. Boglaienko**, B. Tansel

9:30 COLL **48.** Fabricating reservoir micromodels by *in situ* grown calcium carbonate nanocrystals in microfluidic channels. **W. Wang**, S. Chang

9:50 COLL **49.** Effects of confinement and composition on oil/water interface in nanopore environment. **A. Alizadehmojarad**, **L. Vukovic**

10:10 COLL **50.** Impact of microemulsions on mobilization, emulsification, and solubilization of oil in heterogeneous rocks. **T. Qin**, L. Goual

10:30 COLL **51.** Nanoengineering at the oil-water interface to maximize hydrocarbon production. **P.A. Sermon**, G. Georgiades

10:50 COLL **52.** pH-responsive polymer coated nanoparticles for controlled emulsification of heavy oil. **L. Qi**, C. Song, G.J. Hirasaki, R. Verduzco

11:10 COLL **53.** Surfactant Enhanced Oil Recovery (EOR): Role of reservoir wettability and oil-water interfacial tension in designing efficient surfactant systems. **C. Acevedo**, W. Yu, P.D. Patil

11:30 COLL **54.** Formulation and utility of microemulsions in cleaning applications. **C.J. Tucker**, M.H. Keefe, K. Harris

Section H

Moscone Center

2003

Nanoscale Chemical Patterning & Characterization

S. A. Claridge, *Organizer*

W. Liao, *Organizer, Presiding*

8:30 COLL **55.** Biodegradable and biocompatible regular nanopatterned surfaces for selective cell enrichment. **G. Sicilia**, A. Grabowska, I. Notingher, M. Alexander, M. Marlow

8:50 COLL **56.** Tailoring 5–10 nm chemically orthogonal surface patterns on layered materials using sitting phases of polymerizable amphiphiles. **J. Bang**, K.K. Rupp, S.R. Russell, S.W. Choong, T.C. Davis, T. Hayes, A.G. Porter, J.T. Brooks, S.A. Claridge

9:10 COLL **57.** Artificial membranes composed of fluid and polymerizable lipids: Fractional polymerization produces nanoscale domains with retained fluidity and enhanced stability. **S.S. Saavedra**

9:40 COLL **58.** Chemical lift-off lithography and sensors. **W. Liao**

10:10 COLL **59.** Patterning arrays of geometrically complex nanostructures on planar surfaces. **P.S. Cremer**, Z. Zhao, Y. Cai

10:40 COLL **60.** Self-assembly of proteins into periodic nanostructures through spatially-confined nanofluids. **J. Li**

11:10 COLL **61.** Modified soft lithographic approach for Surface-Enhanced Infrared Spectroscopy (SEIRA) substrates and their application to live cell monitoring. **V. Colvin**, N. Taheri, A. Bohoul

11:40 COLL **62.** Characterizing and manipulating mercaptoalkanoic acid molecular ruler multilayers using scanning probe lithography. J.E. Neuman, A.M. Patron, C.P. Causey, **T.J. Mullen**

Section I

Moscone Center

2005

Basic Research in Colloids, Surfactants & Nanomaterials

Colloids

R. Nagarajan, *Organizer*

U. Scheler, *Presiding*

8:30 COLL **63.** Counterion-specific counterion condensation. **U. Scheler**

9:00 COLL **64.** Carbonate rock wettability investigated with finer spatial resolution. O.B. Wani, C. Lai, M. Almahri, M. Chiesa, **S. Al Hassan**

9:20 COLL **65.** Light scattered by hedgehog particles. **J. Bahng**, D. Montjoy, W. Chang, S. Link, N. Kotov

9:40 COLL **66.** Cross-linked cationic diblock copolymer worms are superflocculants for micrometer-sized silica particles. **N. Penfold**, Y. Ning, P. Verstraete, J. Smets, S.P. Armes

10:00 COLL **67.** Spray coating of colloidal and organic layers. W. Ohm, P. Zhang, S. Yu, A. Plech, D. Soderberg, **S. Roth**

10:20 COLL **68.** Elucidating the reactivity and solution dynamics of redox active polymers and colloids. M. Burgess, E. Montoto, K. Hernandez-Burgos, J. Schuh, T. Wei, N. Gavvalapalli, J. Moore, J. Lewis, R. Ewoldt, **J. Rodriguez Lopez**

10:40 COLL **69.** Particle zeta potentials remain finite in saturated salt solutions. **A. Garg**, C. Cartier, K.J. Bishop, D. Velegol

11:20 COLL **70.** Issue of interchangeable use of reactivity assessment assays for nanoparticle colloids in liquid solution. **X. Bi**, P.K. Westerhoff

11:40 COLL **71.** Propagation and separation of charged colloids by cylindrical gel electrophoresis. **D.A. Bikos**, T.G. Mason

12:00 COLL **72.** Morphology and properties of fibers obtained by emulsion electrospinning. **A. Samanta**

Section J

Moscone Center

2007

Deposition & Etching of Nanostructures

Cosponsored by INOR

L. McElwee-White, A. V. Walker, *Organizers*

H. Fairbrother, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL **73.** New strategies for selective deposition of nanoscale materials. F. Minaye Hashemi, D. Bobb-Semple, **S.F. Bent**

9:05 COLL **74.** Using surface chemistry to direct the morphology of thin films and nanoobjects of energy materials. **A.V. Walker**

9:35 COLL **75.** Laser-assisted focused electron beam induced synthesis: Photothermal enhancements to athermal electron beam induced reactions. **P.D. Rack**

10:05 Intermission.

10:20 COLL **76.** Time is of the essence: Using a fourth dimension to improve chemical vapor deposition. **H. Pedersen**

‡ *Cooperative Cosponsorship*

10:50 COLL **77.** Real-time XPS monitoring of atomic layer deposition of HfO_2 on Si surfaces. **P. Shayesteh**, J. Gallet, F. Bournel, J. Schnadt

11:10 COLL **78.** Directed deposition and etching of functional nanostructures using electron beam and plasma irradiation. **C.J. Lobo**

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Sponsored by GEOC, Cosponsored by COLL and ENVR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis, & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Single Crystal Catalysis

Sponsored by CATL, Cosponsored by COLL and WCC

Separation of Macromolecules & Particulates

Sponsored by POLY, Cosponsored by ANYL, COLL and PMSE

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Synthesis of Catalysts by Non-Traditional Methods

Nanoparticle Catalysts

Sponsored by CATL, Cosponsored by COLL and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Theory

Sponsored by CATL, Cosponsored by COLL and ENVR

SUNDAY AFTERNOON

Section A

Moscone Center

2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

M. L. Longo, A. B. Subramaniam, *Presiding*

2:00 COLL **79.** Lipid non-lamellar phases at the solid/liquid interface - structure and dynamics. **T. Nylander**, O. Soltwedel, M. Ganeva, C. Hirst, J. Holdaway, M. Yanez Arteta, M. Wadsater, J. Barauskas, H. Frielinghaus, O. Holderer

2:25 COLL **80.** Stimulus-responsive behavior of giant vesicles consisting of amphiphilic diblock copolymers. **E. Yoshida**

2:50 COLL **81.** Selective blood vessel deletion using liposomes: Studying the effect of liposome composition on *in vivo* behavior. **A. Kros**

3:15 COLL **82.** Physical clotting of blood cells using associating biopolymers as the connective glue: An investigation into the mechanism using optical microscopy. **S.R. Raghavan**

3:40 COLL **83.** Elastic and viscous properties of lipid bilayers: Application of neutron spin echo spectroscopy. **M. Nagao**, E.G. Kelley, R. Ashkar, R. Bradbury, P. Butler

4:05 COLL **84.** Kinetic pathways of self-assembled systems by time-resolved small-angle scattering techniques. **R. Lund**

4:30 COLL **85.** Neutron and x-ray scattering approaches for interdisciplinary structural biology. **T. Forsyth**

4:55 COLL **86.** Opening the SANS toolbox for studying mRNA nanoparticle structure. **C.J. Bowerman**, Y. Xia, J. Chan, C. Clemente, A. Esposito, E. Miracco, B. Kangarlou, M. Nieh, E. Cheung, O. Almarsson

Section B

Moscone Center

2004

Colloidal Nanoparticle Synthesis & Assembly

Y. Sun, S. Wu, *Organizers*

H. Fan, H. Htoon, *Organizers*, *Presiding*

2:00 COLL **87.** Silicon nanocrystal assemblies. **B.A. Korgel**

2:30 COLL **88.** Induction and microwave heating in syntheses of CdSe quantum dots: Effects of extreme high heating rate on their nucleation and growth kinetics. H. Luo, B.A. Kebede, E.J. McLaurin, **V. Chikan**

2:50 COLL **89.** Enhanced emission of nanocrystal solids featuring slowly diffusive excitons. **N.N. Kholmicheva**, M. Zamkov

3:10 COLL **90.** Detecting material state change in surface coated tensile samples using ultrasmall CdSe quantum dots. **T. Frecker**, C. Brubaker, I. Njoroge, G. Jennings, D. Adams, S.J. Rosenthal

3:30 COLL **91.** Ligand-induced freeze of gold nanostars and their SERS activities. **X. Meng**, C. Jiang

3:50 COLL **92.** Chiral inorganic nanostructures. **N. Kotov**

4:20 COLL **93.** Organic nanophotonic materials and devices. **Y. Zhao**

4:50 COLL **94.** Study of Au nanoparticles self-assembly by in-situ transmission electron microscopy. **Y. Liu**, Y. Sun, X. Lin, T. Rajh

5:20 COLL **95.** Synthesis and assembly of plasmonic metal oxide nanocrystals. **D.J. Milliron**

Section C

Moscone Center

2006

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Catalyst Design

Cosponsored by CATL

S. H. Kim, R. M. Rioux, *Organizers*, *Presiding*

2:00 COLL **96.** Dynamic evolution of catalytic surfaces. **C.M. Friend**

2:30 COLL **97.** Metal nanoparticle catalysts based on classically immiscible and metastable alloys. **S.M. Humphrey**, G. Henkelman, P. Kunal, H. Li, H. Guo, G.W. Piburn

3:00 COLL **98.** Catalysis on singly dispersed bimetallic sites. **F. Tao**

3:30 COLL **99.** Ordered bimetallic catalysts for selective hydrogenation and dehydrogenation reactions. **W. Huang**

4:00 COLL **100.** Ideal catalysts beyond single crystals: MOFs with metal oxide-like nodes. D. Yang, V. Bernales, C.J. Cramer, O.K. Farha, J.T. Hupp, L. Gagliardi, **B.C. Gates**

4:30 COLL **101.** Catalyst synthesis by atomic layer deposition. **P.C. Stair**

5:00 COLL **102.** New nanostructures for increased selectivity and stability in catalysis. **F. Zaera**

Section D

Moscone Center

2008

Chemistry & Physics of Tribology

Theoretical & Computational Advances in Tribology

F. Mangolini, *Organizer*

M. Ruths, *Organizer, Presiding*

C. M. Mate, *Presiding*

2:00 COLL **103.** Scale dependence of friction and contact of nanometer to millimeter radius tips. T.A. Sharp, J. Monti, L. Pastewka, **M.O. Robbins**

2:35 COLL **104.** Limits of Lifshitz theory. O. Siles-Brugge, C. Hunter, **G.J. Leggett**, N.H. Williams

2:55 COLL **105.** Effect of load on current across gold-graphite nanocontacts. **A. Martini**, X. Hu, V. Zade, H. Kang, M. Lee

3:30 COLL **106.** Examination of DLC adhesion and wear using MD and in-situ nanoindentation. J.D. Schall, R. Bernal, P. Chen, P. Tsai, Y. Jeng, R. Carpick, **J.A. Harrison**

3:50 COLL **107.** Nonequilibrium molecular dynamics simulations of organic friction modifiers. **J. Ewen**, C. Gattinoni, H. Spikes, N. Morgan, D. Dini

4:10 COLL **108.** Molecular dynamics simulations of multiply alkylated cyclopentane-based lubricant oils. **V. Oklejas**, P.P. Frantz, S.V. Didziulis

4:30 COLL **109.** Dynamics and thermodynamics of lubricants in flow: A molecular and tribological approach. **Y. Guo**, L. di Mare, J. Wong

4:50 COLL **110.** Withdrawn.

Section E

Moscone Center

2010

Coacervation: Physics, Chemistry & Biology

P. L. Dubin, R. Stewart, *Organizers*

Y. Wang, *Presiding*

2:00 COLL **111.** Entropy the assembler (of polyelectrolytes). **J.B. Schlenoff**

2:30 COLL **112.** Simple coacervation of polyguanidiniums and organic polyphosphates. **R. Stewart**, J.P. Jones, G.M. Weerasakare, I. Song

3:00 COLL **113.** Exploring the coacervation/precipitation interface. **P.L. Dubin**, F. Comert, A.J. Malanowski

3:30 COLL **114.** Material dynamics in complex coacervates. **S.L. Perry**

4:00 COLL **115.** Complex coacervation as a dynamic reservoir of intrinsically disordered proteins. **S. Han**

4:30 COLL **116.** Coacervates from biopolymers for cartilage tissue regeneration. Ö. Karabiyik Acar, **A. Kayitmazer**, G. Kose

Section F

Moscone Center

2012

Applied Biosensing Based on Functional Colloids

R. Alvarez Puebla, L. Liz Marzan, W. Parak, J. Sagalés, *Organizers*

G. F. Strouse, *Organizer, Presiding*

2:00 COLL **117.** Plasmonic supercrystals for SERS detection. **R. Alvarez Puebla**

2:30 COLL **118.** Nanoparticles and stem cells, a powerful combination? **W. Parak**

2:50 COLL **119.** Control of primary particle spacing in gold nanoparticle clusters for both high NIR extinction and full reversibility. **E. Moaseri**, B. Changalvaie, T. Truskett, K.P. Johnston

3:10 COLL **120.** Modeling of degradation of virus and amyloid fibril by pre-designed nanoparticles. **S. Sen**, P. Kral

3:30 COLL **121.** Spectroscopic quantification of surface groups on micro- and nanoparticles with conventional and cleavable reporter. T. Behnke, M. Moser, N. Nirmalananthan, **U. Resch-Genger**

4:00 COLL **122.** *In vivo* biomolecule corona onto clinically-used blood-circulating liposomes. **M. Hadjidemetriou**, K. Kostarelos

Section G

Moscone Center

2001

Interfacial Phenomena & the Oil-Water Interface

Financially supported by The Dow Chemical Company

C. Acevedo, C. E. Mohler, C. J. Tucker, *Organizers*, *Presiding*

2:00 COLL **123.** Continuous fabrication of hierarchical and asymmetric bijel structures via Solvent Transfer-Induced Phase Separation (STRIPS). **K.J. Stebe**

2:30 COLL **124.** Molecular structure and bonding at nanoemulsion and planar oil/water interfaces. **G.L. Richmond**

3:00 COLL **125.** Molecular structures of polymer surfaces in different chemical environments. **Z. Chen**

3:30 COLL **126.** Molecular studies of the assembly of co-surfactants at the oil-water interface. **R. Ciszewski**, B. Muller, G. Richmond

3:50 COLL **127.** Mass transfer of lipid-based amphiphiles to water-triglyceride interfaces. **T. Xu**, S.R. Dungan

4:10 COLL **128.** Investigating mass transfer and microstructures formation at liquid/liquid interfaces using FT-IR imaging spectroscopy. **R. Toor**, M. Schmitt, R. Denoyel, M. Antoni

4:30 COLL **129.** Specific anion effects on caffeine partitioning between aqueous and cyclohexane phases. **Y. Zhang**, B.A. Rogers, N.O. Johnson, T.P. Light, T.S. Thompson, G. MacDonald

4:50 COLL **130.** Protein mixture segregation at coffee ring: Real-time imaging of protein ring precipitation by mid-FTIR spectromicroscopy. **S. Choi**, G. Birarda

5:10 COLL **131.** Surface and interfacial exploration of a smooth liquids repellent sol-gel coating. **C. Urata**, A. Hozumi

Section H

Moscone Center

2003

Nanoscale Chemical Patterning & Characterization

S. A. Claridge, *Organizer*

W. Liao, *Organizer, Presiding*

2:00 COLL **132.** Self-assembly in confined spaces: Using defects to advantage. N. Nakatsuka, H. Cao, W. Liao, A. Vaish, T.J. Mullen, P.S. Weiss, **A.M. Andrews**

2:30 COLL **133.** Controlling biomolecular structure and function at the bio/abio interface. **L.J. Webb**

3:00 COLL **134.** Probing nano-environments with high-throughput single-molecule tracking. **D.K. Schwartz**

3:30 COLL **135.** Stable by design: Understanding the role of monomer architecture in stabilizing noncovalent monolayers toward thermal and solvent processing of layered materials. **S.R. Russell**, T. Villarreal, S.A. Claridge

3:50 COLL **136.** Optically directed assembly of colloidal particles. **Y. Zheng**

4:20 COLL **137.** Laser directed crystallization and patterning of methylammonium lead halide perovskites from solution. **S. Chou**, B. Swartzentruber, M.T. Janish, K.C. Meyer, L. Biedermann, S. Okur, B. Burckel, C.B. Carter, B. Kaehr

4:40 COLL **138.** Tarnishing silver into semiconducting hybrid chalcogenides. **J. Hohman**

5:10 COLL **139.** Bottom-up preparation of ordered Rh(I) diisocyanide coordination polymers on gold surfaces and their conductivity and electrochemical stability. **G. Lee**, C.P. Kubiak

Section I

Moscone Center

2005

Nanostructure Engineering & Surface Chemistry for Spectroscopy, Imaging & Alternative Energy Harvesting & Conversion

Financially supported by MilliporeSigma-Energy Materials; CH Instruments, Inc.; The University of Alabama (Chemistry, College of Arts & Science)

N. Hammer, S. Pan, *Organizers*

C. M. Hill, *Presiding*

2:00 COLL **140.** Investigation of charge-transfer complexes between TCNQ and indium phosphide quantum dots. **L. Beck**, E.J. McLaurin

2:20 COLL **141.** Anchoring group affects triplet energy transfer from semiconductor nanocrystals to molecules. **Z. Huang**, X. Li, P. Xia, M.L. Tang

2:40 COLL **142.** Long-range exciton transport in cesium lead halide perovskite nanocrystals organized in ordered nanoscale assemblies. **E. Penzo**, A. Loiudice, E. Barnard, N. Borys, A. Schwartzberg, R. Buonsanti, S. Cabrini, A. Weber-Bargioni

3:00 COLL **143.** Stable n-type thermoelectric multilayer thin films with high power factor from carbonaceous nanofillers. **C. Cho**, C. Yu, J.C. Grunlan

3:20 COLL **144.** Rational design of Bi_2Te_3/graphene quantum dot hybrid nanosheet for enhanced thermoelectric performance. S. Li, T. Fan, X. Liu, J. Luo, F. Liu, H. Meng, **Y. Liu**, F. Pan

3:40 Intermission.

3:50 COLL **145.** Polarized optical spectroscopy of semiconducting polymers in an aligned mesoporous silica system for the study of polaron dynamics. **K. Winchell**, M.E. Voss, B.J. Schwartz, S.H. Tolbert

4:10 COLL **146.** Ultrasensitive probing of the local electronic structure of nitrogen doped carbon and its applications to 2D electronics, catalysis and bio-physics. **S. Lee**, R.A. Mori, B.K. Alpert, M.L. Baker, J. Berry, H. Cho, E. Denison, W.B. Doriese, J.W. Fowler, K.J. Gaffney, B. Gao, J. Gard, G.C. Hilton, K.D. Irwin, Y.I. Joe, S. Kaya, C. Kenney, J. Knight, T. Kroll, D. Li, R. Marks, M. Minitti, K. Morgan, D. Nordlund, G. O'Neil, H. Ogasawara, P. Pianetta, C. Reintsema, T. Schiros, D. Schmidt, D. Sokaras, Y. Song, D.S. Swetz, C. Titus, J. Ullom, T. Weng, C. Williams, A. Wolcott, B.A. Young

4:30 COLL **147.** Probing the local electronic structure of a porphyrin-based single-layer covalent organic framework using STS. **C. Chen**, T. Joshi, H. Li, H. Li, A.D. Chavez, Z. Pedramrazi, J.E. Bredas, W.R. Dichtel, M. Crommie

4:50 COLL **148.** Structure formation, phase behavior, and dynamics of liquid crystals confined to nanopores. **H. Duran**, T. Yildirim, M. Steinhart, H. Butt, G. Floudas

5:10 COLL **149.** NiS doped 3D MoS_2/graphene nanostructured hybrids as high performance hydrodesulfurization catalysts. S. Lonkar, V. Pillai, **S. Al Hassan**

5:30 COLL **150.** Flexible impedance biosensor for folate receptor detection in cancer diagnostic. **J.J. Fuentes-Rivera**, C.R. Cabrera, G. Hernandez

Section J

Moscone Center

2007

Deposition & Etching of Nanostructures

Cosponsored by INOR

H. Fairbrother, L. McElwee-White, *Organizers*

A. V. Walker, *Organizer, Presiding*

2:00 COLL **151.** Deposition of self-assembled monolayers on TiO_2 in air and solution: Implications for photoreactivity and CO_2 photoreduction. **M.A. Hines**, E.S. Skibinski, W.J. DeBenedetti

2:30 COLL **152.** Microplasma-based deposition of functional nanomaterials for energy storage applications. **K.E. Mackie**, M.J. Gordon

2:50 COLL **153.** Deposition of mixed metal nanostructures from bimetallic precursors using electrons: Insights from surface science. **H. Fairbrother**, J.A. Spencer, I. Unlu, R. Kumar, R. Thorman, O. Ingolfsson, S. Barth, K. Johnson, L. McElwee-White

3:20 Intermission.

3:35 COLL **154.** Selectivity in liquid phase etching of III-V materials on the path to developing a gas phase self-limited etching method. **A.J. Muscat**

4:05 COLL **155.** Surface chemistry issues relevant to ALD processes. **F. Zaera**

4:25 COLL **156.** From fundamental electron-induced chemistry to novel unconventional FEBID precursor materials. **J. Warneke**, M. Rohdenburg, G.E. Johnson, J. Laskin, P. Swiderek

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Sponsored by GEOC, Cosponsored by COLL and ENVR

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Single Crystal Catalysis

Sponsored by CATL, Cosponsored by COLL and WCC

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Separation of Macromolecules & Particulates

Sponsored by POLY, Cosponsored by ANYL, COLL and PMSE

Synthesis of Catalysts by Non-Traditional Methods

Model Catalysts, Microporous Materials & Oxides

Sponsored by CATL, Cosponsored by COLL and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Sponsored by CATL, Cosponsored by COLL and ENVR

SUNDAY EVENING

Section A

Moscone Center

Halls B/C

Fundamental Research in Colloids, Surfaces & Nanomaterials

R. Nagarajan, *Organizer*

6:00 - 8:00

COLL **157.** Influence of biomimetic brush nanostructures on the tribology of natural fiber bio-interfaces. **C. Cazeneuve**, J. Vazquez, N. Baghdadli, **G.S. Luengo**

COLL **158.** Coacervation and precipitation in polysaccharide–protein systems. **F. Comert**, A.J. Malanowski, F. Azarikia, P.L. Dubin

COLL **159.** miRNA sensing plasma modified magnetic micromotor. **L. Oksuz**, G. Yurdabak Karaca, F. Kuralay, U. Koc, E. Uygun, A. Uygun Oksuz

COLL **160.** Nanotransformation of vancomycin for overcoming Gram-negative bacteria intrinsic resistance. **J. Hoyo**, K. Ivanova, M. Fernandes, A. Francesko, T. Tzanov

COLL **161.** Fabrication of vanadium oxide thin films from colloidal vanadium oxide (VO_x) nanocrystals for smart window applications. **Y. Jung**, S. Chung

COLL **162.** Organic-inorganic microcapsules via immobilizing bicomponent colloidal particles at oil-water interface. **Y. Wu**, J. Shen

COLL **163.** Templated formation of fullerene stripes with tunable nanometer spacing onto physisorbed monolayers. **C. Fang**, M. Zimmt

COLL **164.** Forming supported lipid multilayers by self-spreading. **T. Liu**, C. Hu, B. Sanii

COLL **165.** Manganese-engineered iron oxide nanocomposites as T_1-T_2 dual-modal contrast agents. **C. Lu**

COLL **166.** Water buffer action under nanoscale confinement studied by fluorescent pH indicator. **J. Fu**, L. Zhang

COLL **167.** Quartz Crystal Microbalance with Dissipation (QCM-D) study of bacterial attachment process on surfaces of different hydrophilicity. **Y. Lee**

COLL **168.** Synthesis of CeO_2 supported noble metal nanoparticles using mixed-valent Mn_3O_4 phase via galvanic replacement reaction. **D. Lee**, I. Lee

COLL **169.** Control of dynamic wetting behaviors on smooth surface for liquid manipulator and slippery surface with multi functionality. **M. Tenjimbayashi**, R. Togasawa, M. Higashi, S. Shiratori

COLL **170.** Anisotropic emission-tuned polymer nanoparticles through a scalable direct approach. **J.D. Ruiz Perez**, S. Mecking

‡ *Cooperative Cosponsorship*

COLL **171.** Biofunctionalized silica-nanopores: Synthesis and characterization by solid state CP-MAS-NMR. **M. Brodrecht**, H. Breitzke, B. Kumari, T. Gutmann, G. Buntkowksy

COLL **172.** Investigation of a nanoscale surface area coverage by a self assembly of amyloidogenic peptides. **P.J. Shevlin**, K. Brown, M. Abdelmalik, A. Olatunbosun, K. Yokoyama

COLL **173.** Investigation of reversible self-assembly of amyloidogenic peptides at nano-scale interface. **J. Battaglia**, **J. Ehret**, M. Endo, A. Islam, K. Yokoyama

COLL **174.** Fabrication of antifreeze infused hydrophilic polymer/nanoparticle composite anti-icing coating for solar cells via spray layer by layer method. **T. Yamazaki**, T. Moriya, T. Matsubayashi, M. Komine, M. Tenjimbayashi, S. Shiratori

COLL **175.** Shea butter infused with natural oils to generate a novel and natural antimicrobial moisturizer. **A. Tremblay**, K. Melkonian, J.I. Rizzo

COLL **176.** Effect of silica size on superhydrophobic property of filter media for water oil/separation. **P. Seeharaj**

COLL **177.** Withdrawn.

COLL **178.** Fabrication of nanoporous carbon as electrodes for supercapacitors. **P. Suwannasarn**, S. Wongkasemjit, T. Chaisuwan

COLL **179.** Silver nanoplate shape control: Use of halide ions to promote vertical growth. **Y. Park**, S. Park, M. Kim

COLL **180.** Luminescent solar concentrators using ZnTe/CdSe/CdS core/shell quantum dots. **A. McDarby**, D. Khon, M. Zamkov

COLL **181.** Infusion of native oils to synthesize novel antimicrobial aurfaces. **K. Velez**, J.I. Rizzo

COLL **182.** Tuning localized surface plasmon resonances in Sn-doped In_2O_3 through radial distribution of dopant atoms and core/shell architectures. **B. Crockett**, A. Jansons, K.M. Koskela, J.E. Hutchison

COLL **183.** Pilot-plant study of using protein to reduce the lipophilic contaminants in paper mills. **A.H. Tayeb**, O.J. Rojas, L. Pal, M. Hubbe

COLL **184.** Unraveling the importance of controlled architecture in bimetallic multilayer electrode toward efficient electrocatalyst. **M. Gu**, B. Kim

COLL **185.** Rational design and fabrication of TiO_2 p-n homojunction for photoelectrochemical and photocatalytic water splitting. **L. Pan**, **G. Shen**, J. Zou, X. Zhang

COLL **186.** Preparation of 2D porous Co_3O_4 nanofoils via graphene mimicking. **T. Han**

COLL **187.** Morphological control of colloidal aluminum nanocrystals. **D. Renard**, C.J. Desantis, B. Clark, M. McClain, N.J. Halas

COLL **188.** Room-temperature formation of Cu-Ag bimetallic heterostructured nanocrystals via galvanic exchange. **W.T. Osowiecki**, X. Ye, A. Alivisatos

COLL **189.** Effect of ZnS on structural and optical properties of $CuInS_2$ quantum dots. **A. Nguyen**, C.D. Heyes

COLL **190.** Combined ionic and hydrogen bonding in polymer multilayer thin film for high gas barrier and stretchiness. **C. Cho**, F. Xiang, J.C. Grunlan

COLL **191.** Direct amination of HPHT ND surfaces for biodetection. **P. Tran**, **E.S. Favre**, **A. Hernandez**, D. Nordlund, A. Wolcott

COLL **192.** Assessment of color strength and pigment stabilization using microencapsulation of anthraquinone dyestuffs with epoxy resin. **S. Liao**

COLL **193.** Control of cesium lead halide perovskite nanocyrstal morphology and photonic properties. **M.J. Jurow**, A. Pan, J. Kang, A. Buyanin, M.A. Koc, M. Salmeron, P. Alivisatos, L. Wang, Y. Liu

COLL **194.** Use of a simple and general approach to modify the surfaces of monodisperse metal oxide nanocrystals with a wide variety of silane coupling agents. **A.W. Jansons**, K.M. Koskela, R. Maust, J.E. Hutchison

COLL **195.** Nano-tribological properties of single monolayers and mixed monolayers of octadecylcarboxylic acid and octacosanoic acid. R. Thomas, L. Clark, T. Perry, E.S. Gawalt, **M. Lim**

COLL **196.** Synthesis and characterization of novel hydrogel beads for selective interactions with carbonaceous nanomaterials. **K.C. Tvrdy**, J. Rowland, N. Sundquist

COLL **197.** Exploration of the growth mechanism of $AgGaS_2$ semiconductor nanoparticles. **S. Paderick**, S. Hughes

COLL **198.** Tuning the optical properties of $AgGaS_2$ nanocrystals. **S. Hughes**, S. Paderick, M. Kessler

COLL **199.** Tunable whiteness coloration behavior on rutile TiO_2 ceramic pigment. **Y. Kim**, R. Yu, J. Yun

COLL **200.** Describing the mechanisms involved in Amot associated membrane binding and fusion. S. Sears, **A.C. Kimble Hill**

COLL **201.** Ferrocene-modified PEI microgels. **N. Sahiner**, S. Demirci, M. Yildiz

COLL **202.** Decrystallization of crystals using gold nano-bullets and the metal-assisted and microwave-accelerated decrystallization technique. **N. Thompson**, Z. Boone-Kukoyi, R. Shortt, C. Lansiquot, B. Kioko, E. Bonyi, K. Aslan

COLL **203.** Tailoring the surface architecture of gold nanoparticles to engage nanoparticle-cell interactions. **K.L. Kinnison**, G.W. Marquart, M.R. Mackiewicz

COLL **204.** Withdrawn.

COLL **205.** Withdrawn.

COLL **206.** Withdrawn.

COLL **207.** Laponite bioactive nanocomposites for orthopedic applications. **J.T. Wilk**, M.E. Hagerman

COLL **208.** Withdrawn.

COLL **209.** Probing the catalytic properties of Ni-based bimetallic phosphides for deep hydrodesulfurization. **P.J. Topalian**, D. Liyanage, S. Brock, M.E. Bussell

COLL **210.** Dabrafenib drug release system based on gold nanoparticle carriers for treatment of melanoma cancer. **L. Running**, R. Espinal, M.R. Hepel

COLL **211.** Controlled release of lenvatinib from multi-functional nanoparticles monitored by surface-enhanced Raman scattering. T. Santiago, **T. Durgan**, M.R. Hepel

COLL **212.** Growth of SiO_2 shells on fluorescent nanodiamond cores for biodetection. **P.J. Sandoval**, **A.A. Len**, **A. Arreola**, D. Nordlund, P. Cigler, A. Wolcott

COLL **213.** Room temperature monolayer ZnS growth on CdS and CdSe cores. **M. Augspurger**, N. Razgoniaeva, M. Zamkov, D. Khon

COLL **214.** Ligand influence on the branching of gold nanocages. **L.M. Bouchet**, J. Bergueiro, E.A. Glitscher, M. Calderon

COLL **215.** Proposing a two-molecule multiplexed neuromorphic system: The first step towards a chemically based artificial brain. N. Nakatsuka, C. Zhao, J. Abendroth, H. Chen, K.M. Cheung, S. Dominik, **L. Scarabelli**, K. Yang, B. Zhu, H. Yang, Y. Yang, M. Stojanovic, P.S. Weiss, A.M. Andrews

COLL **216.** Synthesis of MoS_2/Fe_3O_4 nanocomposites with peroxidase-like activity for applications in H_2O_2 and glucose detection. **V. Nandwana**, W. Huang, E.W. Roth, V.P. Dravid

COLL **217.** Hydrothermal formation of various metal oxides using oxalic acid as a capping agent. **Z. Zander**, D. McCarthy, B.G. DeLacy

COLL **218.** Production and characterization of activated carbon containing polyvinyl alcohol microcapsules. Q.T. Truong, **C.A. Zoto**, N. Orbey, A. Molinaro, J. Ogilvie Battersby

COLL **219.** Single step dipping method of fabricating Fe_3O_4/PVDF-HFP composite porous material for magnetically controllable oil-water separation. **J. Li**, M. Tenjimbayashi, S. Shiratori

COLL **220.** Synthesis and characterization of metallic nanoparticles using dendrimer-templating technology. **S. Merlus**, M.L. Curry, A. Ethridge

COLL **221.** Synthesis and surface properties of poly(methyl methacrylate-butyl acrylate)/polythiourethane core-shell nanoparticles by new click reaction with soap-free emulsion polymerization. **J. Kook**, Y. Kim, K. Hwang, J. Kim, J. Lee

COLL **222.** High density immobilization of oligonucleotides on semiconductor and gold nanoparticles within seconds. **A. Sedighi**, U.J. Krull

COLL **223.** *In situ* synthesis of Ag nanocrystal-embedded metal-organic framework microneedles showing electrical bistability properties. **S. Park**, K. Park, S. Im, M. Kim

COLL **224.** One-step synthesis of silver nanoplates with high aspect ratios: Using coordination of silver ions to enhance lateral growth. **Y. Park**, B. Lee, M. Kim

COLL **225.** Sum-frequency vibrational spectroscopy of electrified water interfaces. **H. Wang**, W. Liu, Y. Shen

COLL **226.** Withdrawn.

COLL **227.** Systematic examination of bimetallic architecture in Pt-Pd nanocatalysts. **J. Legere**, S.E. Skrabalak

COLL **228.** Reporting rotational dynamics of intracellular cargos with Janus particles. **Y. Gao**, S.M. Anthony, Y. Yi, Y. Yu

COLL **229.** Smart colorimetric patches based on plasmonic nanoparticle-decorated thermoresponsive microgels. **A. Choe**, J. Yeom, M. Kim, H. Ko

COLL **230.** Antibacterial layer-by-layer coating of nanoparticles. **K. Ivanova**, A. Ivanova, T.J. Heinze, T. Tzanov

COLL **231.** Optical properties and controllable chiro-optical handedness of symmetric and asymmetric dimer nanocrescents. **P.R. Stevenson**, M. Swartz, C. Coplan, V.A. Tamma, V.A. Apkarian, J.S. Shumaker-Parry

COLL **232.** Peelable temporary coatings by waterborne self-crosslinkable urethane dispersions. **S. Shin**, H. Oh

COLL **233.** Identification of Gram-positive bacterial cell wall components responsible for interactions with cationic nanoparticles. **K. Johnson**, E. Caudill, J.A. Pedersen, C.L. Haynes, V. Feng

COLL **234.** Impact of natural organic matter on the interaction of functionalized diamond nanoparticles with model bacterium *S. oneidensis* MR-1. **J. Kuether**, **R. Tapia Hernandez**, A.C. Mensch, J.A. Pedersen, R.J. Hamers, V. Feng

COLL **235.** Adsorption and decomposition of a chemical warfare agent simulant on copper and molybdenum oxides. **L. Trotochaud**, A.R. Head, R. Tsyshevsky, S. Pletincx, Y. Yu, O. Karslioglu, B.W. Eichhorn, M.M. Kuklja, H. Bluhm

COLL **236.** Withdrawn.

COLL **237.** Encapsulation of responsive liquids in coaxial nanofibers via electrospinning. **J. Lundin**, D. Ratchford, R. Ananth, R. Casalini, J.H. Wynne

COLL **238.** Efficient photocatalytic activity of SnO_2-deposited ZnS nanobelts. J. Lee, J.K. Kim, D. Jeong, **D. Jang**

COLL **239.** Carbon nanomaterials for biomedical applications as antioxidants and drug delivery vehicles. **L.G. Nilewski**, W.K. Sikkema, E.L. Samuel, A.S. Jalilov, K. Mendoza, R. Zhang, R. Huq, C. Beeton, M. Sharpe, D. Baskin, T.A. Kent, J.M. Tour

COLL **240.** Magnetically induced heat generation in magnetic nanoparticles for environmental remediation. **K.J. Coopersmith**, G. Larsen, S. Hunyadi Murph

COLL **241.** Fabrication of Si nanopillar array for ultralow reflectivity. F. Teng, N. Li, L. Liu, D. Xu, **N. Lyu**

COLL **242.** Nucleobase and nucleotide coordinated Au(I/III) nanoparticles for anticancer therapeutics. **Y. Huang**, W. Yeh

COLL **243.** Identification of promising electrografting precursors for the modification of electrode surfaces. **S.E. Shaner**, S.N. Doden, M. Moin, F. Mujid, J.E. Newhouse

COLL **244.** Synthesis and characterization of ceramic-coated α-FeOOH yellow pigments. **Y. Kim**, R. Yu, J. Yun

COLL **245.** Zwitterionic polymers for chronic wound management. K. Ruseva, K. Ivanova, E. Vasileva, **T. Tzanov**

COLL **246.** Solvent free synthesis of nanostructured MoS_2/S-Tio2 photocatalysts for visible light driven water splitting and dye removal. V. Pillai, S. Lonkar, **S. Al Hassan**

COLL **247.** Second harmonic generation studies of indomethacin adsorption to phospholipid membranes. **A.D. Fearon**, G.Y. Stokes

COLL **248.** Targeted detection of mRNA biomarkers using graphene oxide and upconversion nanoparticles. **A. Kanaras**, P. Vilela, A. El-Sagheer, T. Brown, T. Millar, O. Muskens

COLL **249.** Synthesis of large spherical and anisotropic gold nanoparticle dimers using a seeded-growth method. J. Midelet, A. Heuer-Jungemann, A. El-Sagheer, T. Brown, M. Werts, **A. Kanaras**

COLL **250.** Aptamer-gold nanoparticle colorimetric assay evaluation of the role of DNA, small molecule targets, and gold nanoparticle interactions via NMR. **J.E. Smith**, B. Orzech, D. Russel, C. Medley

COLL **251.** Modification of zinc oxide nanoparticles with perfluorophosphonic acids. D. Shoup, **R. Quinones**

COLL **252.** Modification of nitinol nanoparticles with self-assembled alkylphosphonate films. S. Garretson, **R. Quinones**

COLL **253.** Withdrawn.

COLL **254.** Withdrawn.

COLL **255.** Designing a model cell membrane to investigate the absorption of nanoparticles in our skin. **B. Yoder**, A. Sostarecz

COLL **256.** pH-induced conformational switch in novel amide-based amphiphiles and their potential application in liposomes for targeted drug delivery. **C. van Beek**, M. Beltran-Sanchez, N.M. Samoshina, V.V. Samoshin

COLL **257.** Two-dimensional nanoparticle array and cluster formation by supercritical fluid deposition. **J. Wang**, G. Brown, C.M. Wai, S. Apt

COLL **258.** Epoxide chemistry on the Si(100)-(2x1) surface. **J.L. McCracken**, A.J. Pohlman, S.M. Casey

COLL **259.** Targeted delivery of chemotherapeutic drugs and adjuvants using gold nanoparticle carriers. **M. Palmer**, A. Marotta, A. Ortiz, M.R. Hepel

COLL **260.** Static light scattering studies of the aggregation process in the isotropic phase of chromonic surfactants in water. **L.E. Stevenson**, G.R. Van Hecke, K.K. Karukstis

COLL **261.** Withdrawn.

COLL **262.** Highly active cuprous oxide photocathode for the selective photoelectrochemical reduction of carbon dioxide. **S. Alden**, D.A. Rider

COLL **263.** Stabilization and reaction of small molecules on TiO2/Au(111) inverse model catalysts. **J. Wilke**, D. Boyle, D. Schlosser, V.H. Lam, W. Andahazy, A.E. Baber

COLL **264.** Phenothiazine cored poly (aryl ether) dendrons: Phase selective gelation, hydrophobization, oil spill recovery, antiwetting property and formation of fluorescent ink. **N. Lakshmi**

COLL **265.** Synthesis of perfluoro-acrylate-silane co-polymer nanocapsules using emulsifier-free emulsion polymerization: Water-oil repellent and surface properties. **Y. Kim**, J. Kook, K. Hwang, J. Ahn, J. Lee

COLL **266.** Synthesis of lanthanum doped titanate nanotube through a facile hydrothermal route. N. Wongsrisujarit, **M. Hasan**, K. Yeung

COLL **267.** Performance enhancement of fluorescent dyes using nanoparticle encapsulation strategies for LED applications. **X. Ning**, J. Chittigori, Y. Li, G. Horner, R. Sharma, C. Ullal, L. Schadler

COLL **268.** Synthesis of carboplatin like Pt^{2+} complexes with azide and alkyne functionalities for nanomedical applications. **M.T. Wlodarczyk**, O. Camacho-Vanegas, S.A. Dragulska, A. Jarzecki, P.R. Dottino, J.A. Martignetti, A.J. Mieszawska

COLL **269.** Field theory for ligand alignment on nanoparticles: Prospects for self–assembly driven by phase transitions. **P. Satish**, J. Haberstroh, P.L. Geissler

COLL **270.** Delivery of biomolecules into solid-supported lipid bilayers using nanolipoprotein particles. **A. Dang**, M. Coleman, T. Kuhl

COLL **271.** Polyelectrolyte multilayers for controlled FGF-2 release and improved cell attachment on cell culture surfaces. **I. Ding**, A.M. Peterson

COLL **272.** Removal kinetics of 2-Chloroethylethyl Sulphide (CEES) by iron oxide nanoparticles. **S. Kim**, Y. Choe, K. Baek, Y. Lee

COLL **273.** Assembly and disassembly of fluorescent graphene oxide for optical detection of enzymatic activity. **J. Ju**, S. Jeon, T. Kang, H. Kim, M. Kim, S. Lee, J. Kim

COLL **274.** Modification of the surface of zinc oxide nanoparticles in order to increase efficiency of solar cells. **G. Behnke**, R. Quinones

COLL **275.** Alkyl desorption from Si(100)-2×1 by nonadiabatic hydrogen elimination. **A. Pohlman**, D. Kaliakin, S.A. Varganov, S.M. Casey

COLL **276.** Aqueous multiphase emulsion droplets as cellular mimics: Production and utilization. **C. Crowe**, P. Torre, R. Poudyal, P.C. Bevilacqua, S.S. Mansy, C.D. Keating

COLL **277.** Novel DNA origami structure for Doxorubicin delivery. **S. Palazzolo**, V. Kumar, C. Russo Spena, M. Hadla, S. Bayda, G. Corona, V. Canzonieri, G. Toffoli, F. Rizzolio

COLL **278.** Label-free detection and quantification of specific proteins in complex biological fluids through clogging in cellulose paper. **J. Pazzi**, M. Xu, W. Cheung, A.B. Subramaniam

COLL **279.** Paper-based growth of liposomes and proteoliposomes using PAPYRUS in ionic buffers. **M. Xu**, A.B. Subramaniam

COLL **280.** Photochemical study of silver nanoparticles formed from the reduction of silver ions by humic acid. **R. Leslie**, D. Pullman

COLL **281.** Nanoparticle system based on tripeptide oil in water emulsion to deliver Au nanocrystals and taxol for cancer therapy. **S.A. Dragulska**, M.T. Wlodarczyk, R. Ulijn, A.J. Mieszawska

COLL **282.** Decoupling mechanisms of palladium nanoparticle synthesis on a biotemplate. **E. Retzlaff-Roberts**, O. Adigun, G. Novikova, L. Wang, B. Kim, J. Ilavsky, J. Miller, S. Loesch-Fries, M.T. Harris

COLL **283.** Direct correlation of atomic structure and emission dynamics in single colloidal core/shell nanostructures. **K.R. Reid**, J.R. McBride, S.J. Rosenthal, J. Macdonald, A.D. LaCroix

COLL **284.** Effect of fluctuations on excited state rates in core/shell quantum dots. **A. Balan**, H. Eshet, J.H. Olshansky, E. Rabani, A. Alivisatos

COLL **285.** Adsorption and decontamination of alpha-synuclein from medically and environmentally-relevant surfaces. **H. Phan**, S.L. Bartelt-Hunt, J.C. Bartz, J. Ayers, B. Giasson

COLL **286.** Effects of ice-binding proteins from cold-adapted insect *Tenebrio molitor* on calcite crystallization. **A. Kishishita**, J. Lugo, X. Wen

COLL **287.** Characterization of ordered naphthalene diimide films deposited in soils substrates from floating films at the air-water interface. **J. Dillenburger**, A. Muenter Edwards, J. Reczek

COLL **288.** Investigations of cationic gemini surfactants by NMR relaxation and diffusion. **B.J. Schepergerdes**, S.J. Bachofer, M.D. Lingwood

COLL **289.** Modular approach for the attachment of protein domains to the exterior of the P22 virus-like particle scaffold. **D. Patterson**, M. Hicks, M. Terra, B. Western, P. Krugler, T. Douglas

COLL **290.** Zinc chalcogenide nanostructures as flame retardant coatings. **Y. Wang**, T. Athauda, Y. Vasquez, Q. Wang

COLL **291.** Withdrawn.

COLL **292.** Giant Nanocrystal Quantum Dots (gNQDs) as Förster Resonance Energy Transfer (FRET) donors. **M. Chern**, T. Nguyen, A. Mahler, A.M. Dennis

COLL **293.** Advances in correlating the optical and structural behavior of single quantum dots. **N. Orfield**, J.R. McBride, N. Mishra, S.M. Click, S. Majumder, H. Htoon, J.A. Hollingsworth

COLL **294.** Potential of indium tin oxide nanoparticles to produce reactive oxygen species in environmental systems as a result of Sn level and location. **J. Grundy**, C. Ngan, N.B. Saleh, L.E. Katz, M. Kirisits, C. Saez Cabezas, D.J. Milliron

COLL **295.** Effect of micelle polydispersity on first order phase transitions in polyelectrolyte-colloid systems. **D. Marco**, P.L. Dubin

COLL **296.** Modification of magnetite nanoparticle surface through Sn_2 substitution of the hydroxide functional group with a chloride group. **I. Rios Cruz**, **P. Velez Vega**, **C. Beauchamp Perez**, **G.E. Alvarez**, **T. Massas Le'Cleres**, F. Roman, V. Fernandez-Alos, O. Perales

COLL **297.** Asymmetric silica encapsulation toward colloidal Janus nanoparticles: Concave nanoreactor for template-synthesis of electocatalytic hollow Pt nanodendrite. **J. Koo**, D. Kim, K. Jin Goo, I. Lee

COLL **298.** Functional interphases based on peptidomimetic-coated gold surfaces. **C. Sugnaux**, A. Kelleghan, P. Messersmith

COLL **299.** pH-responsive Fenton reaction performing polymeric micelles: Applications in anticancer and antibacterial therapy. **D. Yoo**, J. Noh, E. Jung, D. Lee

COLL **300.** Potential of nontoxic materials to treat dentinal hypersensitivity and promote tooth remineralization. **A.D. Fritza**, K. Rashwan, B. Karels, G. Sereda

COLL **301.** Substitution effects in aniline on electrochromic properties of hybrid flexible device. **A. Uygun Oksuz**, E. Eren, C. Alver, G. Yurdabak Karaca

COLL **302.** Removal of car batteries heavy metals contaminants from aqueous solutions with composite chitosan/alginate coated magnetite beads. **K.M. Molina**, V. Fernandez-Alos, F. Roman

COLL **303.** Antitumoral activity of (-)-epicatechin loaded chitosan nanoparticles *in vitro* and *in vivo*. **A. Perez Ruiz**, I. Olivares Corichi, F. Ganem Rondero, J. Suarez Sandoval, J. García Sánchez

COLL **304.** Morphology-controlled self-assembly and synthesis of photocatalytic nanocrystals. **Y. Zhong**, J. Wang, F. Bai

COLL **305.** Morphology-controlled synthesis and metalation of porphyrin nanoparticles with enhanced photocatalytic performance. **J. Wang**, Y. Zhong, F. Bai

COLL **306.** Investigation into the synthesis and oxidative toxicity associated with colloidal C_{60} nanoparticles. **S. Irving**, K. Shumard, K.D. Ausman

COLL **307.** Study on protein conformation and bio-activity of antibodies immobilized on varied nanofibrous membranes. **C. Zhao**, Y. Deng, B. Pan, Y. Si, G. Sun

COLL **308.** Microfluidic multifunctional capacitive sensors using ionic liquid electrodes and CNT/PDMS composites for simultaneous sensing of pressure and temperature. S. Yoon, **S. Chang**

COLL **309.** Surface modification of conductive polymer thin films by femtosecond laser direct writing. **S. Chae**, J. Choi, H. Kim

COLL **310.** Photothermal heating of nanoparticles for activation of initiators for radical polymerization. **T.M. Steeves**, R.C. Steinhardt, A. Esser-Kahn

COLL **311.** Ambient STM study of sequentially adsorbed octanethiol and biphenylthiol monolayers on Au(111). **G. Avila-Bront**

COLL **312.** Rotating disk electrode characterization of soluble redox active polymers for use in nonaqueous redox flow batteries. **J. Davila**, K. Hernandez-Burgos, E. Montoto, J. Moore, J. Rodriguez Lopez

COLL **313.** Synthesis of WS_2 by low-pressure chemical vapor deposition. Z. Luo, J. Qian, Z. Sun, **D. Zhang**

COLL **314.** Effect of substituents on anthracene transmitters on triplet transfer from CdSe nanocrystals. **P. Xia**, Z. Huang, X. Li, J.J. Romero, V.I. Vullev, G.S. Pau, M.L. Tang

COLL **315.** X-ray imaging observation of interfacial changes between epoxy and metal particles during thermal curing. **S. Lee**, Y. Kim, H. Lee, H. Kim, D. Noh

COLL **316.** Effects of OH and Cl adsorption on the surface structure of α-Fe_2O_3: A density functional theory study. **Q. Pang**, H. DorMohammadi, O. Isgor, L. Arnadottir

COLL **317.** Solid-liquid equilibrium of binary mixtures with curved interface. **F. Liu**, L. Zargarzadeh, H. Chung, J.A. Elliott

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COLL **318.** Peptide loaded microgels as antimicrobial surface coatings. **L. Nyström**, R. Nordstrom, G. Frenning, B. Saunders, R. Álvarez-Asencio, M.W. Rutland, M. Malmsten

COLL **319.** Coexisting coacervate systems to model aqueous phase separated compartments in biology. **G.A. Mountain**, C.D. Keating

COLL **320.** Responsive nanogels as carriers for antimicrobial peptides. **R. Nordstrom**, L. Nyström, B. Saunders, M. Malmsten

COLL **321.** Withdrawn.

COLL **322.** Three dimensional (3D) plasmonic hot spot for label-free sensing and effective photothermal killing of multiple drug resistant superbugs. **S.J. Jones**, S.S. Sinha, A. Pramanik, P.C. Ray

Section B

Moscone Center

Halls B/C

Colloidal Nanoparticle Synthesis & Assembly

H. Fan, H. Htoon, Y. Sun, S. Wu, *Organizers*

6:00 - 8:00

COLL **323.** Asymmetric and multi-compartment polymersomes as structural analogues of eukaryotic cells. **A. Peyret**, E. Ibarboure, S. Lecommandoux

COLL **324.** Assessing the influence of oxidizing agents when preparing colloidal spinel-type $MgMn_2O_4$ nanocrystals. **G. Nolis**, J. Bolotnikov, J. Cabana

COLL **325.** Hollow silica particles: Measurement of mechanical stability through mercury porosimetry, and development of a low cost, scalable process for hollow silica. **J. Lasio**, F. Woerner, A. Allgeier, C. Chan, J.D. Londono

COLL **326.** Polyampholyte microgels: From molecular design to ionic traps and switches. **A. Pich**, W. Xu

COLL **327.** Tannin-mediated layer-by-layer assembly of titania nanocrystals for efficient UV-protective colloidal materials. **H. Son**, B. Koo, J. Lee, K. Kim, J. Jang, M. Yoon, J. Cho, J. Kim, Y. Nam

COLL **328.** Withdrawn.

COLL **329.** Development of supramolecular particles made from guanosine derivatives to study and modulate the immune system. **M. Acosta Santiago**, S.E. Quiñonez González, J.M. Rivera

COLL **330.** Fabrication and characterization of platinum coated with solution processed graphene. **Y. Zhang**

COLL **331.** Electron microscopy in color: Revealing chemical complexity in emergent nanocrystal systems utilizing advanced STEM-EDS. **J.R. McBride**, K. Reid, S.J. Rosenthal

COLL **332.** Hybrid lipid-coated silver nanoparticles differentially shielded from Ag^+ release. **M.R. Mackiewicz**, T.J. Miesen

COLL **333.** Gadolinium oxide nanocrystals as T_1 MRI contrast agents: Balancing colloidal stability with surface accessibility. **V. Colvin**, N. Taheri, G. Stinnett, R. Paultler, P. Decuzzi, I. Al-Dhahir, A. Mendoza-Garcia

COLL **334.** Engineering a thermoresponsive nanogel with a photothermal core for cancer cell specific binding. **Z. Yu**, D. Tang, K.J. Shea, X. Qi, H. Gu

COLL **335.** Magnetic nanocapsule: A novel theranostic agent in biomedicine. **V. Nandwana**, A. Singh, J. Higham, M.M. You, T.S. Zheng, S. Shankar, V.P. Dravid

COLL **336.** Using molecular dynamics to investigate the effect of intra- and inter-strand hydrogen bonding on sequence-chirality specific adsorption of single-stranded DNA (ssDNA) onto Single-Walled Carbon Nanotubes (SWCNTs). **K. Hinkle**, F.R. Phelan

COLL **337.** Chiroptical responses of helical arrays of plasmonic nanoparticles around anisotropic nanopillars. **A. Jung**, C. Kim, B. Yeom

COLL **338.** Solution-processed photovoltaic devices utilizing Semiconductor Excitonic Nanoshells (SENS). **N. Razgoniaeva**, M. Zamkov

COLL **339.** Hybrid nano-antibacterials to control biofilm-associated infections. **K. Ivanova**, J. Hoyo, T. Tzanov

COLL **340.** Withdrawn.

COLL **341.** Oxidation state dependence of capping agent for site-selective silica coating of gold nanorods. **J.G. Hinman**, J. Eller, J. Li, J. Li, C.J. Murphy

COLL **342.** Precisely tuning size, dopant incorporation, and radial distribution of dopants in metal oxide nanocrystals via a continuous, living growth synthesis. **A.W. Jansons**, B. Crockett, K.M. Koskela, J.E. Hutchison

COLL **343.** Biopolymer hydrogels embedded with lignin-silver nanocomposites with broad activity against antibiotic-resistant clinical isolates. **T. Tzanov**, P. Petkova, K. Ivanova, N. Slavin, H. Bach, I.S. Stefanov

COLL **344.** Microwave-assisted synthesis and characterization of nanomaterials. **P.N. Njoki**, P. Nwokogu, T. Williams, R. Yehdego

COLL **345.** Nitrogen enriched hierarchically nanoporous carbon derived from one-pot sol-gel synthesis of polybenzoxazine precursor for CO_2 capture and storage. **T. Chaisuwan**, S. Wongkasemjit, N. Manmuanpom

COLL **346.** Occlusion of sulfate-based diblock copolymer nanoparticles within calcite: Effect of varying the surface density of anionic stabilizer chains. **S.P. Armes**, Y. Ning

COLL **347.** Core@Shell architecture: Enhancing catalytic performance. **K. Koczkur**, J. Legere, D. Chen, E.W. Harak, S.E. Skrabalak

COLL **348.** Biocatalytic synthesis and characterization of ultra-long-chain fatty acid sugar alcohol monoesters. **Z. Guo**

COLL **349.** Interaction of size-tailored PEGylated iron oxide nanoparticles with lipid membranes and cells. **N. Gal**, A. Scheberl, A. Lassenberger, L. Herrero Nogareda, E. Reimhult

COLL **350.** Aqueous synthesis, characterization and optimization of novel nanostructures for water purification. **T. Eldred**, J.C. Poler

COLL **351.** MRI reporter contrast agents for ultrasound ablative therapy. **J. Wang**, J. Yang, G. Anthony, S. Sammet, W.C. Trogler, A. Kummel

COLL **352.** *Sapindus mukorossi* fruit extract mediated synthesis of silver nanoparticle and study of its catalytic and antibacterial activity. **A. Mitra**, G. Dinda, D. Halder, N. Pal, C. Vazquez Vazquez, M. Lápez-Quintela

COLL **353.** Autocatalytic sol-gel synthesis of organic-inorganic hybrid material. **R. Francis**, G.P. Gopalan

COLL **354.** Synthesis and adsorption studies of quaternized magnetic cellulose nanocomposite as adsorbent for hexavalent chromium removal. **J. Wanathammapong**, T. Witoon, K. Kasemwong

COLL **355.** Hybrid microemulsion (uE)/sol-gel chemistry to synthesize and harvest $CaTiO_3$:Cr^{3+} NIR nanophosphors. **P.A. Sermon**, J. Eloi

COLL **356.** Effects of the template removal methods and pH on formation of hierarchical porous silica using natural rubber as template. **C. Phattharachindanuwong**, N. Hansupalak, C. Warakulwit, J. Plank, Y. Chisti

COLL **357.** Miniaturised continuous processing units for rapid synthesis and purification of liposomes. **N. Dimov**, E. Kastner, Y. Perrie, N. Szita

COLL **358.** Nanoparticle synthesis and harvesting from W/O microemulsions (uE). **P.A. Sermon**, M. Worsley, J. Eloi

Section C

Moscone Center

Halls B/C

Basic Research in Colloids, Surfactants & Nanomaterials

R. Nagarajan, *Organizer*

6:00 - 8:00

COLL **359.** Platonic micelles: A novel aggregation behavior of sulfonatocalix[4]arene-based micelles. **S. Fujii**, K. Sakurai

COLL **360.** Visible light photoactivity of 1-D TiO_2 by targeted decoration of transition metal nanodots. **M. Hasan**, S. Ferdousi, K. Yeung

COLL **361.** Effects of osmolytes on caffeine partitioning thermodynamics. **T.S. Thompson**, A.P. Allsbrook, Y. Zhang

COLL **362.** Elucidating distinct Au(111) and TiO_2/Au(111) surface sites for the selective oxidation of ethanol to acetaldehyde. **D. Boyle**, J.A. Wilke, V.H. Lam, A.E. Baber

Section D

Moscone Center

Halls B/C

Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment

A. H. Flood, S. L. Tait, *Organizers*

6:00 - 8:00

COLL **363.** Tuning dynamic two-dimensional supramolecular self-assemblies at surfaces by molecular design. **H.D. Castillo**, J. Dobscha, J.M. Espinosa Duran, S. Kim, S. Debnath, Y. Liu, D.C. Ashley, Y. Serada, B. Hirsch, M. Baik, D. Lee, K. Raghavachari, P. Ortoleva, A.H. Flood, S.L. Tait

COLL **364.** Controllable self-assembly of peptoid material. **F. Jiao**, H. Jin, P. He, C. Chen, J.J. De Yoreo

COLL **365.** Towards the design, synthesis, and characterization of the self-assemblies of shape-persistent tricarb macrocycles. **J. Dobscha**, H.D. Castillo, Y. Liu, J.M. Espinosa-Duran, S. Debnath, Y. Sereda, K. Raghavachari, P. Ortoleva, S.L. Tait, A.H. Flood

COLL **366.** Self-assembly of designed helical-repeat protein on mica characterized using atomic force microscopy. **S. Zhang**, H. Pyles, D. Baker, J.J. De Yoreo

COLL **367.** Rapid electro-formation of robust and transparent biopolymer gels in prescribed shapes. **A. Gargava**, H. Mani, S.R. Raghavan

COLL **368.** Synthetic lipids for liposome derivatization, targeting and triggered release towards drug delivery applications. **M. Best**, A.M. Bayer, S. Alam, S. Whitehead

COLL **369.** Interfacial carbene reactions on hard and soft material interfaces. **A. Shestopalov**

COLL **370.** Carboranethiol self-assembled monolayers on gold surfaces. N. Sohrabnia, A. Yavuz, A. Yilmaz, **M. Danisman**

COLL **371.** Withdrawn.

Section E

Moscone Center

Halls B/C

Deposition & Etching of Nanostructures

Cosponsored by INOR

H. Fairbrother, L. McElwee-White, A. V. Walker, *Organizers*

6:00 - 8:00

COLL **372.** Interfacial stress induced metal thin film surface reorganization. **J. Chen**, I. Tevis, M. Thuo

COLL **373.** Size and aging effects on antimicrobial efficiency of silver nanoparticles coated on polyamide fabrics activated by atmospheric DBD plasma. **A. Zille**, M. Fernandes, A. Francesko, T. Tzanov, M. Fernandes, F. Oliveira, L.M. Almeida, A.P. Souto, N. Carneiro, T. Amorim, M.F. Esteves

COLL **374.** Hot Splash Coating (HSC): A method to create thin layers of doped carbon on metal surfaces. M.R. Alves, **R. Silva**

Section F

Moscone Center

Halls B/C

Nanoscale Chemical Patterning & Characterization

S. A. Claridge, W. Liao, *Organizers*

6:00 - 8:00

COLL **375.** Control of surface energy to optimize post CMP cleaning efficiency for microelectronics fabrication. S. Ozbek, T. Walker, **G. Basim**

Section G

Moscone Center

Halls B/C

Interfacial Phenomena & the Oil-Water Interface

Financially supported by The Dow Chemical Company

C. Acevedo, C. E. Mohler, C. J. Tucker, *Organizers*

6:00 - 8:00

COLL **376.** Self-propelled ionic gel at air-water interface. **K. Furukawa**, T. Teshima, Y. Ueno

MONDAY MORNING

Section A

Moscone Center
2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

K. Gawrisch, N. Malmstadt, *Presiding*

8:30 COLL **377.** Lipid phase separation enhances fusion. **Z. Imam**, L.E. Kenyon, G. Ashby, M. Mendicino, F. Nagib, J.C. Stachowiak

8:50 COLL **378.** Molecular interactions between model cell membranes and nanoparticles. **Z. Chen**

9:15 COLL **379.** Phospholipid flippases of the human erythocyte. S. Cook, M. Hosek, J. Lyles, J. Paterson, S. Smriti, M.L. Zimmerman, **D.L. Daleke**

9:40 COLL **380.** Exploring the interactions of transition metal ions with lipid membranes. **P.S. Cremer**, M. Poyton, X. Cong, A. Sendecki, S. Pullanchery, A. Baxter, S. Sun

10:05 COLL **381.** Model system for separating viral membrane binding and fusion. **S.G. Boxer**, R. Rawle, P. Kasson, E. Webster

10:30 COLL **382.** Stochastic molecular mechanisms in membrane traffic. **J. Stachowiak**

10:55 COLL **383.** Blue fluorescent amino acid for studying membrane protein structure and dynamics. **F. Gai**

11:20 COLL **384.** Novel application of cellulose paper as a platform for fabricating giant liposomes. K. Kresse, M. Xu, J. Pazzi, M. Garcia-Ojeda, **A.B. Subramaniam**

11:45 COLL **385.** Investigating the mechanism of electromechanical coupling in voltage-gated ion channels by time-resolved x-ray & neutron interferometry. **J.K. Blasie**

Section B

Moscone Center
2004

Colloidal Nanoparticle Synthesis & Assembly

H. Htoon, Y. Sun, S. Wu, *Organizers*

H. Fan, *Organizer, Presiding*

Z. Jiang, *Presiding*

8:30 COLL **386.** Enriching Ag nanocrystals with gold. **D. Qin**, X. Sun, Y. Wu

9:00 COLL **387.** Configurational behavior and charge correlation of Zwitterionic brushes at the solid-water interface. **W. Chen**, J. Mao, J. Yu, M.V. Tirrell

9:30 COLL **388.** Shape switchable patchy particles. **X. Zheng**, D. Pine, M. Weck

9:50 COLL **389.** General strategy for assembling metal chalcogenide capped semiconductor nanocrystals into open, mesoporous films with precisely controlled properties. **J. Ondry**, S. Robbennolt, Y. Yan, E. Harr, H. Kang, S.H. Tolbert

10:10 COLL **390.** Reversible self-assembly of monodisperse gold nanoparticle clusters in aqueous solution via pH-tunable interactions between surface ligands. **E. Moaseri**, B. Changalvaie, J. Bolinger, L. Johnson, T. Truskett, K.P. Johnston

10:30 COLL **391.** Two-dimensional bipyramid plasmonic nanoparticle superstructure with four distinct orientational packing orders. **Q. Shi**

10:50 COLL **392.** Watching nanoparticle growth with tandem *in situ* SAXS-XAS. **T. Li**

11:20 COLL **393.** Multimodal resonant soft x-ray scattering for soft materials. **C. Wang**

11:50 COLL **394.** Self-assembly of two-dimensional nanoparticle superlattice membranes: A study by synchrotron x-ray scattering. **Z. Jiang**

Section C

Moscone Center
2006

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Soft Interfaces

Cosponsored by CATL

S. H. Kim, R. M. Rioux, *Organizers*, *Presiding*

8:30 COLL **395.** Investigations of water structure at lipid interfaces. **P.S. Cremer**, S. Pullanchery, S. Sun

9:00 COLL **396.** Interactions of surfactants and polyelectrolytes at water surface studied by surface tension and phase-sensitive sum frequency generation. **K. Chou**

9:30 COLL **397.** Biomedical surface analysis: Recent advances and opportunities for characterizing immobilized proteins and functionalized gold nanoparticles. **D.G. Castner**

10:00 COLL **398.** Surface-modified nanoparticles for biomedical imaging. **P. Chen**

10:30 COLL **399.** Structure and function of surface immobilized peptides and enzymes in air. **Z. Chen**

11:00 COLL **400.** *In-situ* surface spectroscopy and imaging: From electrocatalytic to live cell interfaces. **D.H. Gracias**

Section D

Moscone Center
2008

Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment

S. L. Tait, *Organizer*

A. H. Flood, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 COLL **401.** Hierarchical self-assembly of functionalized tricarbazolo triazolophane macrocycles at the liquid-solid interface. **H.D. Castillo**, J. Dobscha, B. Hirsch, Y. Liu, J.M. Espinosa-Duran, S. Debnath, Y. Serada, K. Raghavachari, P. Ortoleva, A.H. Flood, S.L. Tait

9:00 COLL **402.** Predicting crystalline structures of organic photovoltaic materials involving alkoxybenzonitriles via multiscale computer-aided design. **J.M. Espinosa Duran**, H.D. Castillo, J. Dobscha, S. Debnath, S.L. Tait, A.H. Flood, K. Raghavachari, P. Ortoleva

9:20 COLL **403.** First-principles modelling of supramolecular organic assembly driven by electrostatic interactions. **A. De Vita**

9:50 COLL **404.** Electronic effects in the self-assembly of strong donor/acceptor mixtures on metal surfaces. **R. Otero**

10:20 COLL **405.** Playing with electrons: How physics meets organic chemistry in the engineering of molecular interfaces. **W. Hofer**

10:50 COLL **406.** Electronic structure of two-dimensional pi-conjugated networks: Impact of lattice symmetry. **J.E. Bredas**

11:20 COLL **407.** Tuning charge transport in supramolecular assemblies of porphyrins on Au. **J.D. Batteas**

11:50 COLL **408.** Entropic intermixing in a binary molecular system: A two-dimensional hydrogen-bonded molecular substitutional solid solution. **J. MacLeod**, J. Lipton-Duffin, D.F. Perepichka, F. Rosei

12:10 COLL **409.** Self-assembly under confinement: Nanocorrals for understanding fundamentals of 2D crystallization. **L. Verstraete**, J. Greenwood, B. Hirsch, S. De Feyter

Section E

Moscone Center
2010

Coacervation: Physics, Chemistry & Biology

P. L. Dubin, *Organizer*

R. Stewart, *Organizer, Presiding*

8:30 COLL **410.** Build-up and breakdown of a cytoskeleton in complex coacervate synthetic cells. J. Groen, E. Te Brinke, **E. Spruijt**, W. Huck

9:00 COLL **411.** Actin encapsulation and assembly in polypeptide coacervates. **S. Srivastava**, P. McCall, S.L. Perry, D. Kovar, M. Gardel, M.V. Tirrell

9:30 COLL **412.** Cell-like structures by coacervation: Polymer microcapsules with addressable inner compartments that can harbor biomolecules, colloids or microbial species. **S.R. Raghavan**, A. Lu, W.E. Bentley

10:00 COLL **413.** Protein coacervation in the processing of biomolecular composites. **A. Miserez**, B. Gabryelczyk, C. Hao

10:30 COLL **414.** Alternative solvent for biology. T. Nott, T. Craggs, P. Farber, J. Forman-Kay, **A. Baldwin**

11:00 COLL **415.** Measuring the intracellular dew point: Phase transitions in cells. **C. Brangwynne**

Section F

Moscone Center
2012

Applied Biosensing Based on Functional Colloids

R. Alvarez Puebla, W. Parak, J. Sagalés, G. F. Strouse, *Organizers*

L. Liz Marzan, *Organizer, Presiding*

8:30 COLL **416.** Designing bio-functionalised colloids for biosensing. **M. Stevens**

9:00 COLL **417.** Functionalizing iron oxide with genomic DNA: Materials for drug capture. **C. Blumenfeld**, M.D. Schulz, S. Hetts, R.H. Grubbs

9:20 COLL **418.** Silica coated ferrimagnetic nanoparticles in trace glycoprotein recovery for LC-MS. **N. Sortedahl**, E.J. Rodriguez, P. Wei, Y. Hua, D.A. Egas, M.J. Wirth

9:40 COLL **419.** Synthesis, characterization and functionalization of inorganic, water soluble nanoparticles. **J. Huehn**, N. Feliu, W. Parak

10:00 COLL **420.** Interpreting sensing mechanisms in nucleic acid-wrapped nanotube sensors through computational approaches. **A. Alizadehmojarad**, A. Beyene, E.G. Tindall, M.P. Landry, **L. Vukovic**

10:20 COLL **421.** Fluorescent nanodiamond labelled with gold nanoparticles for enhanced optical and electron microscopy imaging. **W. Liu**, T. Weil

10:40 COLL **422.** Understanding the interaction of nanoparticles and cells. **N. Feliu**, W. Parak

Section G

Moscone Center
2001

Interfacial Phenomena & the Oil-Water Interface

Financially supported by The Dow Chemical Company

C. Acevedo, C. E. Mohler, C. J. Tucker, *Organizers*, *Presiding*

8:30 COLL **423.** Amphiphilic block copolymers at the oil-water interface. **P. Alexandridis**

9:00 COLL **424.** Dynamic and thermodynamic factors controlling transient Marangoni flow at the oil/water interface under convective diffusion surfactant adsorption conditions. **R.D. Tilton**, G. Duner, S. Garoff, T.M. Przybycien

9:30 COLL **425.** Dynamics of oil-water interfaces: Adsorption, polymerization, and transport. **T. Squires**

10:00 COLL **426.** Formation of multi-nanoemulsions for colloidal synthesis. M. Zhang, P. Malo de Molina, **M.E. Helgeson**

10:30 COLL **427.** Exploring the interfacial synergy between polymers and surfactants. **B. Schabes**, C. Steen, G. Richmond

10:50 COLL **428.** Pickering nanemulsions using bespoke sterically-stabilized diblock copolymer nanoparticles. **S.P. Armes**

11:10 COLL **429.** One-step formation of stable multiple emulsions. **P.M. Guenoun**, M. Protat, N. Bodin, N. Pantoustier, J. Daillant, F. Gobeaux, F. Malloggi, P. Perrin

11:30 COLL **430.** Microemulsion interfacial tension and characteristic length scale model using a microscopic curvature approach and the HLD concept. **V. Torrealba**, R.T. Johns

11:50 COLL **431.** Determining the dynamic interfacial tension during droplet/bubble generation using T-junction and co-flowing microchannels. **K. Wang**, X. Wang, L. Yang, G. Liu, G. Luo

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Section H

Moscone Center

2003

Nanoscale Chemical Patterning & Characterization

S. A. Claridge, W. Liao, *Organizers*

S. Claridge, *Presiding*

8:30 COLL **432.** Generation of patterned multifunctional surfaces using orthogonal click chemistries. **K. Brooks**, J. Yatvin, C.D. McNitt, R.A. Reese, C. Jung, V. Popik, J.J. Locklin

8:50 COLL **433.** Bioinspired interfaces with controlled anisotropic wetting at scales <10 nm for ultrathin patterned films. **S.W. Choong**, S.R. Russell, J. Bang, J.O. Bechtold, J.K. Patterson, S.A. Claridge

9:10 COLL **434.** Programming polymer nanoarchitectures by DNA origami technology. **Y. Tokura**, Y. Jiang, A. Welle, M.H. Stenzel, K.M. Krzemien, J. Michaelis, R. Berger, C. Barner-Kowollik, Y. Wu, T. Weil

9:30 COLL **435.** Polymer pen chemical lift-off lithography. **X. Xu**, Q. Yang, K.M. Cheung, C. Zhao, N. Wattanatorn, J.N. Belling, J. Abendroth, L. Slaughter, C.A. Mirkin, A.M. Andrews, P.S. Weiss

9:50 COLL **436.** Nanoimprint lithography using DNA nanostructure templates. **H. Liu**

10:20 COLL **437.** Bottom-up approach to high density array of patterned polymer brushes. **P. Gopalan**

10:50 COLL **438.** Surface assembly and packing preferences of fibrinogen mediated by the periodicity and alignment of block copolymer nanodomains. **J. Hahm**, T. Xie, A. Vora, P.J. Mulcahey, C. Liu, D.P. Sanders

11:20 COLL **439.** Monolayer assembly of polyaromatics by shear-induced alignment and by 2D porous networks. **C. Chen**

Section I

Moscone Center

2005

Nanostructure Engineering & Surface Chemistry for Spectroscopy, Imaging & Alternative Energy Harvesting & Conversion

Financially supported by MilliporeSigma-Energy Materials; CH Instruments, Inc.; The University of Alabama (Chemistry, College of Arts & Science)

N. Hammer, S. Pan, *Organizers*, *Presiding*

8:30 COLL **440.** Actuatable DNA origami-nanoparticle composites for energy harvesting and storage. A. Dehankar, J. Johnson, C. Castro, **J.O. Winter**

8:50 COLL **441.** Studies of electrochemical reactions at individual nanostructures via combined electroanalytical and optical methods. **C.M. Hill**

9:20 COLL **442.** Nanoelectrochemical techniques for high-resolution imaging and characterization of catalytic nanostructures. **M.V. Mirkin**, T. Sun, M. Zhou, Y. Yu, D. Wang, H. Xin

9:50 COLL **443.** Detecting small molecule binding with membrane proteins. **N. Tao**

10:20 Intermission.

10:30 COLL **444.** Gold nanoparticle assisted delayed luminescence in conjugated polymers. **L. Rothberg**, R. Chakraborty

11:00 COLL **445.** Growth of highly fluorescent gold and silver nanoclusters. D. Mishra, F. Aldeek, G. Palui, **H.M. Mattoussi**

11:30 COLL **446.** Competitive partial charge transfer interactions with hydrogen-bonded solvent networks. **N. Hammer**

Section J

Moscone Center

2007

ACS Award in Colloid Chemistry: Symposium in honor of Nicholas A. Kotov

P. Podsiadlo, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL **447.** Colloidal assembly in alchemical space. **S.C. Glotzer**

9:05 COLL **448.** Control of DNA-functionalized nanoparticle assembly. **M. Olvera De La Cruz**

9:35 COLL **449.** Large-scale nanocrystal arrays. **P. Mulvaney**, C. Kinnear, H. Zhang, A. Roberts, T. James, J. Cadusch

10:05 Intermission.

10:15 COLL **450.** Surface patterning of nanoparticles with polymer patches. **E. Kumacheva**

10:45 COLL **451.** Can particles mimic atoms and molecules? **Z. Nie**, C. Yi, S. Zhang, Y. Yang

11:15 COLL **452.** Stimuli-responsive materials by nanoscale assembly and disassembly. **Y. Yin**

11:45 Concluding Remarks.

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Sponsored by GEOC, Cosponsored by COLL and ENVR

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Nanocatalysis

Sponsored by CATL, Cosponsored by COLL and WCC

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Functional Lignocellulosics & Nanotechnology

Tuning Interfacial Phenomena with Ligno-Nanocellulosic Materials

Sponsored by CELL, Cosponsored by CARB and COLL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Sponsored by CATL, Cosponsored by COLL and ENVR

MONDAY AFTERNOON

Section A

Moscone Center

2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, N. Srividya, *Organizers*

A. N. Parikh, *Organizer, Presiding*

J. Stachowiak, *Presiding*

2:00 COLL **453.** Development of a porous photocatalytic matrix for encapsulation of membrane-bound proteins. **K.E. Johnson**, S. Gakhar, S.H. Risbud, M.L. Longo

2:20 COLL **454.** Time-resolved second harmonic microscopy of molecular transport through living cell membranes. **H. Dai**

2:45 COLL **455.** Chemical imaging of the lipid composition at the site of influenza budding. **M.L. Kraft**, A.N. Yeager, P.K. Weber, J. Zimmerberg

3:10 COLL **456.** Modulating effects of small molecules on the structure and dynamics of lipid-membranes. **X. Cheng**

3:35 COLL **457.** Crowding-induced mixing of lipid bilayers: Examination of mixing energy, reversibility, and dynamics. **M.L. Longo**

4:00 COLL **458.** Effects of defects on lipid biomembranes. **M. Nieh**, Y. Xia, F. Heberle, J. Katsaras

4:25 COLL **459.** Super-resolution stimulated emission depletion-fluorescence correlation spectroscopy reveals nanoscale membrane reorganization induced by pore-forming proteins. N. Kumar Sarangi, I. Ilangumaran Ponmalar, S. Visweswariah, J. Kumar Basu, **G.K. Ayappa**

4:50 COLL **460.** Nanosafety and toxicity assessment by using sponteous beating cardiomyocytes. **S. Zou**

Section B

Moscone Center

2004

Colloidal Nanoparticle Synthesis & Assembly

H. Htoon, Y. Sun, S. Wu, *Organizers*

H. Fan, *Organizer, Presiding*

O. Chen, *Presiding*

2:00 COLL **461.** Epitaxially connected quantum dot superlattices. **T. Hanrath**, F. Wise, L. Kourkoutis, F. Escobedo, K. Whitham, B. Savitzky

2:30 COLL **462.** Nanocube superlattices of $CsPbBr_3$ perovskites and pressure-induced phase transformation at atomic and mesoscale levels. **O. Chen**, Y. Nagaoka, K. Hills-Kimball, R. Tan, R. Li, Z. Wang

3:00 COLL **463.** Self-assembly of actinyl peroxide nanoclusters with cationic surfactant. **Y. Gao**, J. Szymanowski, T. Zhang, P.C. Burns, T. Liu

3:20 COLL **464.** Stimuli-responsive colloidal architectures and porous membranes by melt-shear organization. **S. Vowinkel**, D. Scheid, M. Gallei

3:40 COLL **465.** Framework stability vs. collapse: Quantifying the role of nearest-neighbor nanocrystal bonding as a key factor in determining order in mesoporous colloidal nanocrystal frameworks. **T.E. Williams**, D. Ushizima, P. Ercius, C. Zhu, D.J. Milliron, B. Helms

4:00 COLL **466.** Assembly of free-standing, flexible, citrate-capped gold nanoparticle films at the air-water interface. **L. Beecher**, J.J. Houlihan, V.A. Apkarian, J.S. Shumaker-Parry

4:20 COLL **467.** Complex superparamagnetic particle architectures: Obtaining novel properties by controlled assembly and combination of nano-building-blocks to nanostructured entities. **K. Mandel**

4:40 COLL **468.** Nanoparticles, nanorods and shish-kebabs with precisely controlled dimensions, compositions, and architectures. **Z. Lin**

5:10 COLL **469.** Synthesizing dual-emitting quantum dots on indium phosphide cores. **A.M. Dennis**, R. Toufanian, M. Chern, T. Nguyen, A. Mahler

Section C

Moscone Center

2006

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Catalysts for Selective Chemical Transformations

Cosponsored by CATL

S. H. Kim, R. M. Rioux, *Organizers*, *Presiding*

2:00 COLL **470.** Biomimetic catalysis in green organic transformations. **J.E. Backvall**

2:30 COLL **471.** Fischer-Tropsch synthesis on cobalt catalysts-on the effect of water revisited. **A. Holmen**, E. Rytter

3:00 COLL **472.** Aspects of the Fischer Tropsch reaction mechanism in the light of chemical transient kinetics. **N. Kruse**

3:30 COLL **473.** Selective hydrocarbon oxidation catalysis by Au atomic and nanoclusters. **H. Kung**, M.C. Kung

4:00 COLL **474.** Probing the role of particle size in nickel phosphide hydrotreating catalysts. **M.E. Bussell**, P.J. Topalian, D. Liyanage, S. Brock

4:30 COLL **475.** Competing forces in chiral surface chemistry: Enantiospecific adsorption versus enantiomer self-aggregation. **A.J. Gellman**, Y. Yun

5:00 COLL **476.** Hot electron-mediated surface chemistry on solid-gas and solid-liquid interfaces. **J. Park**

Section D

Moscone Center

2008

Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment

A. H. Flood, *Organizer*

S. L. Tait, *Organizer, Presiding*

2:00 COLL **477.** Chemisorption impacts on physisorption: Perturbations of 2D self-assemblies at the liquid-solid interface. **B. Hirsch**, A. Braganca, J. Greenwood, O. Ivasenko, T. Phan, S. De Feyter

2:20 COLL **478.** Nanoconfined self-assembly on a grafted graphitic surface under electrochemical control. **T. Huynh**, T. Phan, O. Ivasenko, S. F. L. Mertens, S. De Feyter

2:40 COLL **479.** Surface-confined molecular nanostructures: Influencing molecule-surface interactions as well as electronic surface properties. **M. Stoehr**

3:10 COLL **480.** Hierarchical assembly of Xe atoms in an atomically precise array of quantum boxes. **T. Jung**, L.H. Gade, M. Stoehr, J. Lobo Checa, J. Bjoerk, E. Ortega, E. Meyer, S. Kawai, S. Nowakowska, A. Waeckerlin

3:40 COLL **481.** Templated 2D supramolecular assembly of fullerenes on graphite by five-coordinate gallium–porphyrin monolayers. **J. Kamm**, M.D. Hopkins

4:00 COLL **482.** Supramolecular control of interfacial structure in organic semiconductors. **D.F. Perepichka**

4:30 COLL **483.** Hierarchical self-assembly of novel organic polycyclic aromatic molecular systems into 1D and 2D nanomaterials. **H.P. Rathnayake**, H. Sims, J. Sharpensteen, P. Chinnappan

4:50 COLL **484.** Adsorption of n-alkanes on the surface of h-boron nitride: A thermodynamic and molecular dynamics study. **N.A. Strange**, J.Z. Larese

5:10 COLL **485.** Multiscale and hierarchical organic materials by design, synthesis, and self-assembly. **A.H. Flood**, J. Dobscha, H.D. Castillo, J.M. Espinosa-Duran, Y. Sereda, S. Debnath, K. Raghavachari, P. Ortoleva, S.L. Tait

Section E

Moscone Center

2010

Coacervation: Physics, Chemistry & Biology

P. L. Dubin, R. Stewart, *Organizers*

S. L. Perry, *Presiding*

2:00 COLL **486.** Resistance to cold cataract in the eye lens proteins of a cold-adapted fish. **R.W. Martin**, J. Bierma, A. Ledray, A. Kiss

2:30 COLL **487.** Design and optimization of polyphosphate coacervates for use in biomedical devices. **M. Filiaggi**, A. Momeni

3:00 COLL **488.** Complex coacervate for cardiac regeneration. **Y. Wang**

3:30 COLL **489.** Discovery of a family of new LCST peptide polymers: Coacervation behavior and self-assembly. **A. Chilkoti**

4:00 COLL **490.** Engineering Pickering emulsions using protein/polysaccharide complexes. **Q. Huang**

4:30 COLL **491.** Functionality of protein-polysaccharide hydrogels. **S.L. Turgeon**, X. Le, C.J. Souza, L. Rioux

5:00 COLL **492.** Using coacervation to achieve surface-selective particle deposition. **L. Piculell**

Section F

Moscone Center

2012

Applied Biosensing Based on Functional Colloids

L. Liz Marzan, W. Parak, J. Sagalés, G. F. Strouse, *Organizers*

R. Alvarez Puebla, *Organizer, Presiding*

2:00 COLL **493.** Super Temporal-Resolved Microscopy (STReM) for measuring fast interfacial dynamics. **C.F. Landes**

2:30 COLL **494.** New luminescence nanothermometers in different biological windows. **f. Diaz**, O. Savchuk, J. Carvajal, M. Aguilo

3:00 COLL **495.** Improving surgery via selective detection of ovarian tumors using fluorescent nanoparticles. **J.M. Berlin**

3:30 COLL **496.** Liver specific MRI contrast agents based on Mn^{2+} containing nanoparticles. **I. Lee**

4:00 COLL **497.** Targeted sensing and drug delivery using smart nanoparticles. A. Heuer-Jungemann, A. El-Sagheer, P. Lackie, T. Brown, **A. Kanaras**

Section G

Moscone Center

2001

Interfacial Phenomena & the Oil-Water Interface

Financially supported by The Dow Chemical Company

C. Acevedo, C. E. Mohler, C. J. Tucker, *Organizers*, *Presiding*

2:00 COLL **498.** Strategies for making smart foams, emulsions and multiphasic gels stabilized by functional particles. **O.D. Velev**

2:35 COLL **499.** Probing hydrophobic interactions at solid/water/oil/air interfaces and surface interaction mechanisms of deformable emulsion droplets. **H. Zeng**, A. Faghihnejad, C. Shi, L. Zhang, L. Xie, J. Huang, X. Cui

3:05 COLL **500.** Ion specific effects in Winsor III microemulsions. B. Trotter, M. Kadhum, B.J. Shiau, **J.H. Harwell**

3:35 COLL **501.** How molecular structure of surfactants determine the dynamics and viability of wettability alteration. S. Das, Q. Nguyen, **R.T. Bonnecaze**

4:05 COLL **502.** Effects of salinity on oil recovery: Experimental and theoretical studies of crude oil-water-calcite surface restructuring and associated physical and (electro) chemical interactions. **J.N. Israelachvili**, S. Chen, Y. Kaufman, D. Seo, A. Schrader, K. Kristiansen, H. Dobbs, N. Cadirov, J. Boles

4:35 COLL **503.** Simple-to-apply wetting model to predict the thermodynamically stable and the metastable contact angles on textured/rough/pattered surfaces. **Y. Kaufman**, S. Chen, H. Mishra, A.M. Schrader, D. Lee, S. Das, J.N. Israelachvili

4:55 COLL **504.** Molecular and colloidal phenomena at aqueous interfaces of structured oils. **N.L. Abbott**

Section H

Moscone Center

2003

Nanoscale Chemical Patterning & Characterization

S. A. Claridge, W. Liao, *Organizers*

S. Claridge, *Presiding*

2:00 COLL **505.** New dimensions in patterning: Placement and metrology of chemical functionality at all scales. **P.S. Weiss**

2:30 COLL **506.** Construction of highly ordered surface molecular nanostructures: From non-covalent interaction to covalent bond. D. Wang, **L. Wan**

3:00 COLL **507.** Chemical orthogonality at the molecular limit: Structural lessons from the membrane applied to layered material interfaces. **S.A. Claridge**

3:30 COLL **508.** Controlling molecular self-assembly on graphene and graphite at the nanoscale: Combining bottom-up and top-down strategies. **S. De Feyter**

4:00 COLL **509.** Surface mass spectrometry and STM characterizations of compositionally patterned monolayers and their post-assembly chemical modifications. **M. Zimmt**, J. He, C. Fang, R.A. Shelp, O. Fejfar

4:30 COLL **510.** Subsurface structure fingerprint of 2D materials and heterostructures by their nanomechanical response. Q. Tu, B. Lange, H. Kim, Y.G. Yingling, V. Blum, **S. Zauscher**

4:50 COLL **511.** Quantitative connections between Raman spectroscopy and scanning tunneling microscopy in chemisorption on graphite. **A. Brown**, B. Hirsch, P. Walke, S. De Gendt, S. De Feyter

5:10 COLL **512.** Chemisorption on graphitic substrates imaged at the single molecule level. **B. Hirsch**, A. Braganca, K. Tahara, T. Ishikawa, Y. Tobe, M. Melle-Franco, S. De Feyter

Section I

Moscone Center

2005

Nanostructure Engineering & Surface Chemistry for Spectroscopy, Imaging & Alternative Energy Harvesting & Conversion

Financially supported by MilliporeSigma-Energy Materials; CH Instruments, Inc.; The University of Alabama (Chemistry, College of Arts & Science)

N. Hammer, S. Pan, *Organizers*, *Presiding*

2:00 COLL **513.** Optically transparent ultramicroelectrode for studying local electrochemical events of single Au nanoparticle using combined methods of electrochemistry and dark field scattering microscopy. **Y. Ma**, S. Pan

2:20 COLL **514.** Structural plasmonics studied using ultrafast spectroscopy beyond the diffraction limit. **K.L. Knappenberger**

2:50 COLL **515.** Directional charge-separation in organic semiconductor nanowire crystals. **M. Barnes**

3:20 COLL **516.** Long-range catalytic communications within and between single nanocatalysts. **P. Chen**

3:50 Intermission.

4:00 COLL **517.** Observation of local redox events at individual plasmonic nanoparticles using spectroelectrochemistry methods. **S. Pan**

4:30 COLL **518.** Photophysical investigation of electron ejection efficiencies of novel organic near-IR absorbing dyes into TiO_2 based semiconductor surfaces for dye-sensitized solar cell applications. **L.E. McNamara**, H. Cheema, J.H. Delcamp, N. Hammer

4:50 COLL **519.** Mechanistic insights into multiple blinking states in small core-shell and core-multishell quantum dots. **C.D. Heyes**

5:10 COLL **520.** Organo-Metal Halide (OMH) Perovskite Quantum Dots (PQDs): Effective surface passivation using peptides. **J.Z. Zhang**

Section J

Moscone Center

2007

ACS Award in Colloid Chemistry: Symposium in honor of Nicholas A. Kotov

P. Podsiadlo, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 COLL **521.** Non-additive interactions at chemically and structurally complex interfaces. **N.L. Abbott**

‡ *Cooperative Cosponsorship*

2:35 COLL **522.** Programmable materials from DNA bonds and nanoparticle atoms. **C.A. Mirkin**

3:05 COLL **523.** Nanoparticle assembly: Bridging size scales and dimensionalities. **M. Niederberger**

3:35 Intermission.

3:45 COLL **524.** Making all the puzzle pieces fit: Shape directed assembly of anisotropic nanocrystals into multi-component superlattices. **C.B. Murray**, T. Paik, N.J. Greybush, Y. Wu, S. Najmr, C.R. Kagan

4:15 COLL **525.** Synthetic methodology for colloidal synthesis of inorganic nanomaterials: Limitations and opportunities. V. Srivastava, I. Fedin, H. Zhang, **D.V. Talapin**

4:45 COLL **526.** Building materials from colloidal nanoparticles. **L. Cademartiri**

5:15 Concluding Remarks.

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Nanocatalysis

Sponsored by CATL, Cosponsored by COLL and WCC

Janus Particles: Synthesis, Characterization & Applications

Sponsored by PMSE, Cosponsored by COLL and MPPG‡

Functional Lignocellulosics & Nanotechnology

Modification & Analytics

Sponsored by CELL, Cosponsored by CARB and COLL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Mechanistic Studies of Catalysis in Photocatalytic & Photoelectrodes

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms

Sponsored by CATL, Cosponsored by COLL and ENVR

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

R. Nagarajan, *Organizer*

8:00 - 10:00

11, 31, 44, 107, 135, 139, 145, 160-162, 165-166, 168-170, 178, 182-183, 187-188, 192-194, 200, 202, 215, 218, 221-222, 227-229, 231, 235, 239-240, 243, 246, 248, 257, 264, 267-271, 275-276, 280-281, 284, 290, 293-294, 298, 306-307, 310, 314, 316, 323, 338, 388, 417, 420, 466, 511. See previous listings.

593-594, 665, 699. See subsequent listings.

TUESDAY MORNING

Section A

Moscone Center

2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

D. L. Daleke, C. Naumann, *Presiding*

8:30 COLL **527.** Pattern recognition of membrane images to deduce cellular signaling status. **G. Liu**, Y. Liu, D. Hanna, M. Lohrer

8:55 COLL **528.** Spontaneous phospholipid membrane formation by histidine ligation. **A. Bhattacharya**, N.K. Devaraj

9:15 COLL **529.** Hydrogel-assisted membrane protein reconstitution for studying GPCR dependence on lipid composition. **N. Malmstadt**

9:40 COLL **530.** Dimerization of a GPCR in membranes investigated by SANS. O. Soubias, J. Nickels, W.E. Teague, Jr., K.L. Weiss, K.G. Hines, J. Katsaras, **K. Gawrisch**

10:05 COLL **531.** Toward a quantitative continuum model for membrane shape fluctuations. **F.L. Brown**

10:30 COLL **532.** Interfacing proteins with *de novo* membrane formation. **N.K. Devaraj**

10:55 COLL **533.** Hybrid model membrane combining micropatterned lipid bilayer and hydrophilic polymer brush. **K. Morigaki**, T. Nishimura, F. Tamura, Y. Tanimoto, K. Ando, Y. Sudo, F. Hayashi, Y. Iwasaki

11:20 COLL **534.** pH-dependent behavior of lipid bilayer coatings on mesoporous silica nanoparticles. **D.Y. Sasaki**, C. Ashley, E. Carnes, S. Sankhagowit, C. Ting

11:45 COLL **535.** Investigating electrostatic interactions between PIP_2 and the EphA2 receptor tyrosine kinase. X. Shi, S. Christie, R. Lingerak, G. Gilmore, P.G. Rodriguez, J. Muller-Greven, M. Buck, B. Wang, **A.W. Smith**

Section B

Moscone Center

2004

Colloidal Nanoparticle Synthesis & Assembly

Y. Sun, S. Wu, *Organizers*

H. Fan, H. Htoon, *Organizers*, *Presiding*

8:30 COLL **536.** Designed nanoparticles architectures by self-assembly. **O. Gang**

9:00 COLL **537.** Exploring plasmon-exciton coupling at the surface of TiO_2 nanorods. **B.G. DeLacy**, D. McCarthy, Z. Zander, Y. Rao, H. Fang, H. Dai

9:30 COLL **538.** Room temperature, scalable cation exchange in PbS and CdSe quantum dots using a silver(I) complex. A.L. Morris, W.R. Tilluck, S.E. Benjamin, C. Lin, H. Hamo, E. Lozano, **P.G. Van Patten**

9:50 COLL **539.** Controlled assembly of metallic nanoaggregates and their use in understanding cell uptake of nanoparticles. **J.M. Berlin**

10:10 COLL **540.** Synthesis and assembly of gold nanoparticles/polymers: Spheres, prisms, octadehra, and rods…oh my! **S.M. Budy**, D. Hamilton, Y. Cai, M.K. Knowles, S.M. Reed

10:30 COLL **541.** Transforming layered to nonlayered two-dimensional materials: Cation exchange of SnS_2 to Cu_2SnS_3. **Y. Wang**, Y.V. Morozov, M. Zhukovskyi, R. Chatterjee, S. Draguta, P. Tongying, S. Rouvimov, M.K. Kuno

10:50 COLL **542.** DNA-assembled chain-like nanoparticle architectures with tailorable organizations. **C. Tian**, M. Cordeiro, D. DiMarzio, M. Liu, H. Xin, J. Lhermitte, C. Ma, O. Gang

11:10 COLL **543.** Fabrication and application of inorganic nanoparticle superstructures. **Z. Tang**

11:40 COLL **544.** Synchrotron-based x-ray techniques for in-situ superlattice discovery and processing of nanocrystal assembles. **Z. Wang**

Section C

Moscone Center

2006

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Surface Science of Functional Interfaces

Cosponsored by CATL

S. H. Kim, R. M. Rioux, *Organizers*, *Presiding*

9:00 COLL **545.** Functionalizing surfaces with polymeric layers. **N.D. Spencer**

9:30 COLL **546.** Alkyl-cyclens as effective sulfur- and phosphorus-free additives in engine oils for improved boundary lubrication. **Y. Chung**, Q.J. Wang, T.J. Marks, M. Delferro, M. Desanker, J. Lu, X. He

10:00 COLL **547.** When surfaces get rough: Studies of the assembly and frictional properties of SAMs and graphene SAM-composites on surfaces with nanoscale roughness. **J.D. Batteas**

10:30 COLL **548.** Depositing nanostructures using electron beams: Insights from surface science. **H. Fairbrother**

11:00 COLL **549.** Surface structure dependence in oxide catalysis: Comparison of methanol reaction on CeO_2 oriented surfaces and nano crystallites. **S.H. Overbury**

11:30 COLL **550.** Water speciation and mechanochemical reactions at/in multicomponent silicate glass surfaces. **S.H. Kim**

Section D

Moscone Center

2008

Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment

S. L. Tait, *Organizer*

A. H. Flood, *Organizer, Presiding*

8:30 COLL **551.** Topochemical synthesis of a two-dimensional polymer *via* [2+2] cycloaddition on the multigram scale. **R. Lange**, G. Hofer, T. Weber, N. Juergensen, U. Lemmer, G. Hernandez-Sosa, D. Schlueter

8:50 COLL **552.** Structure elucidation of two-dimensional polymers synthesized at the air/water interface. **V. Mueller**, F. Shao, M. Moradi, R. Lange, R. Zenobi, T. Jung, B.T. King, D. Schlueter

9:10 COLL **553.** Self-assembly and on-surface polymerization of bromine-functionalized pyrene derivatives on noble metal surfaces. **B. Tran**, **T. Pham**, **F. Song**, **M. Nguyen**, **M. Kivala**, **M. Stoehr**

9:30 COLL **554.** Charged induced formation of crystalline network polymers. A.A. Raja, D. Kim, S. Subramanian, **C.T. Yavuz**

9:50 COLL **555.** Exploring molecular assembly at surfaces. **F. Rosei**

10:20 COLL **556.** Hierarchy of interactions and templation effects in supramolecular assembly at surface: From organic monolayers to thin films. **G. Costantini**

10:50 COLL **557.** Sophisticated photoresponsive system made of supramolecular assembly of photochromic diarylethene at solid/liquid interface. **K. Matsuda**

11:20 COLL **558.** Understanding intermolecular interactions driving the self-assembly of alkoxybenzonitriles on graphene. **S. Debnath**, **J.M. Espinosa-Duran**, **J. Dobscha**, H.D. Castillo, S.L. Tait, A.H. Flood, P. Ortoleva, K. Raghavachari

11:40 COLL **559.** Stimuli responsive phase behavior in hydrogen-bonded bicomponent supramolecular networks. **G. Velpula**, J. Teyssandier, K.S. Mali, S. De Feyter

12:00 COLL **560.** Structural transformations and self-assembly of interfacial methanol ice on hydrophobic surfaces. **D. Yang**, X. He

Section E

Moscone Center

2010

ACS Award for Research at an Undergraduate Institution: Symposium in honor of Maria Hepel

S. Andreescu, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL **561.** Electroanalytical characterization of environmental chemical processes of engineered nanoparticles. A. Karimi, K. Kirk, **E. Andreescu**

8:55 COLL **562.** Search for new properties and applications of micro- and nanohydrogels. M. Karbarz, E. Zabost, K. Kaniewska, M. Mackiewicz, K. Marcisz, **Z. Stojek**

9:15 COLL **563.** Quasi-adiabatic proton exchange membrane fuel cell fixture for automotive cold-starts. **C.A. Rice**, A.O. Pistono

9:35 COLL **564.** Nanocarbon bowls: Functionalization, structures, applications. **M.A. Petrukhina**

9:55 Intermission.

10:10 COLL **565.** Functionalized porous organometallic compounds as inhibitor of cell division. S. Bashir, B. Martinez, **J.L. Liu**

10:30 COLL **566.** Relationship between phosphorous and metals in Lake Auburn. **A. Bazilio**

10:50 COLL **567.** Characterization of three pathogenic L-ferritin mutants that cause neuroferritinopathy. **F. Bou-Abdallah**

11:10 COLL **568.** Thread- and paper-based devices for use in enzyme assays for Point-of-Care (POC) diagnostic devices. A. Gonzalez, M. Gaines, C. Liu, L. Estala, **F.A. Gomez**

11:30 COLL **569.** Modification of the paper-based NanoCerac antioxidant assay for high-throughput use: An analysis of twenty-four green teas for antioxidant activity throughout six consecutive infusions. **E. Sharpe**, F. Hua, S. Schuckers, E. Andreescu, R. Bradley

Section F

Moscone Center

2012

Applied Biosensing Based on Functional Colloids

R. Alvarez Puebla, W. Parak, J. Sagalés, G. F. Strouse, *Organizers*

L. Liz Marzan, *Organizer, Presiding*

8:30 COLL **570.** Genome-wide DNA methylation variations upon engineered nanomaterials and their implications in nanosafety assessment. **S. Liu**

9:00 COLL **571.** Catalytic enhancement of multienzyme cascades co-localized on colloidal quantum dots. **J. Vranish**, M. Ancona, E. Oh, I. Medintz

9:20 COLL **572.** Antibiofouling manganese oxide nanoparticles: Synthesis, characterization, and potential applications for T_1-weighted MR imaging of tumors. **X. Shi**, P. Wang, J. Yang, B. Zhou, Y. Hu, F. Xu, L. Xing, M. Shen, G. Zhang

9:40 COLL **573.** Quantum dot (QD)-fullerene (C_{60}) conjugates for imaging real-time changes in cellular membrane potential. **O.K. Nag**, M. Stewart, A. Huston, J. Delehanty, A. Efros, K. Susumu, P. Dawson

10:10 COLL **574.** Cerium oxide nanoparticles as novel biosensing tools: Properties, sensing mechanism and applications. A. Othman, G. Bulbul, A. Hayat, **E. Andreescu**

10:30 COLL **575.** GlycoNanoparticle barcodes for pathogen identification. **M.I. Gibson**

Section G

Moscone Center

2001

Chemistry & Physics of Tribology

Lubricants & Lubrication: From Macro to Nano

M. Ruths, *Organizer*

F. Mangolini, *Organizer, Presiding*

J. Yu, *Presiding*

8:30 COLL **576.** Friction and lubrication from the nano (molecular) through the micro (μm-mm) to the macro (geological) scales, and over large time and velocity scales. **J.N. Israelachvili**

9:05 COLL **577.** Nanorhelogy of complex fluids at interfaces: Bulk behavior and complex slip length. **B. Cross**, C. Barraud, F. Restagno, E. Charlaix

9:25 COLL **578.** Binary and ternary systems with ionic liquids in confinement. M. Han, **R.M. Espinosa-Marzal**

9:45 COLL **579.** Shear banding of piezoviscous fluids as a stability problem. B. Galmiche, **L. di Mare**, J. Wong

10:05 COLL **580.** Local rheology of lubricants. **J. Wong**

10:25 COLL **581.** Anomalous spreading kinetics of polymer lubricant films. **C.M. Mate**, B.A. Noble, B. Raeymaekers

10:45 COLL **582.** Quantitative analysis of Raman spectra of fatty acid lubricants under pressure. R.X. Rammeloo, K. Guha, **C.D. Bain**

11:05 COLL **583.** Controlling friction and adhesion using two-dimensional responsive microgels. **S. Giasson**

11:25 COLL **584.** Interfacial properties of fluid lubricants on bearing material surfaces. **J.M. Helt**

11:45 COLL **585.** Formulation chemistry for ultra-stable ester-based oils. **T.E. Karis**

12:05 COLL **586.** Relation between adsorption and nanoscale tribological performance of organic friction modifiers. A. Pham, P. Nalam, V. Castillo, B. Thiebaut, **R.M. Espinosa-Marzal**

Section H

Moscone Center

2003

Deposition & Etching of Nanostructures

Cosponsored by INOR

L. McElwee-White, A. V. Walker, *Organizers*

H. Fairbrother, *Organizer, Presiding*

8:30 COLL **587.** Plasma-assisted atomic layer deposition for energy conversion and storage devices. **M. Creatore**

9:00 COLL **588.** Tin alkyls as a tin source in hybrid molecular beam epitaxy. T. Wang, R.P. Harkins, A. Prakash, C.J. Cramer, B. Jalan, **W.L. Gladfelter**

9:20 COLL **589.** Evidence for surface-plasmon-mediated precursor dissociation in ultrashort-pulsed-laser-induced surface chemistry. **S. Randolph**, M. Straw, A. Botman, J. Filevich

9:50 Intermission.

10:05 COLL **590.** Metalorganic chemical vapor deposition of 2D materials: Challenges and new approaches. **J. Redwing**

10:35 COLL **591.** Atomic Layer Etching (ALE) using sequential thermal reactions: Atomic Layer Deposition (ALD) in reverse. **S.M. George**, Y. Lee, J. DuMont, N. Johnson, D. Zywotko

10:55 COLL **592.** Sequential infiltration synthesis for nanoscale patterning. **J. Elam**, S.B. Darling, Y. Tseng, Q. Peng, M. Biswas, J. Libera, A. Mane, L. Ocola

Section I

Moscone Center

2005

Nanostructure Engineering & Surface Chemistry for Spectroscopy, Imaging & Alternative Energy Harvesting & Conversion

Financially supported by MilliporeSigma-Energy Materials; CH Instruments, Inc.; The University of Alabama (Chemistry, College of Arts & Science)

N. Hammer, S. Pan, *Organizers*

S. Pan, *Presiding*

8:30 COLL **593.** Insight into the recombination kinetics of colloidal silicon nanocrystals. **S. Brown**, J.B. Miller, E. Hobbie

8:50 COLL **594.** Simultaneous time-dependent surface enhanced Raman spectros-copy, metabolomics and proteomics reveal cancer cell death mechanisms associated with Au-nanorod photo-thermal therapy. **Y. Wu**, M.R. Ali, M.A. El-Sayed

9:10 COLL **595.** Synthesis of gold nanoprism with dual effects of plasmon resonance and non-linear optical property to improve the performances of organic solar cell. **B. Gong**, Y. Tai

9:30 COLL **596.** Three dimensionally assembled gold nanostructures for visible light-driven water oxidation. **H. Son**, Y. Nam

9:50 Intermission.

10:00 COLL **597.** Plasmon-coupled resonance energy transfer: A real-space real-time computational electrodynmaics approach. **W. Ding**, L. Hsu, G.C. Schatz

10:20 COLL **598.** Development and molecular understanding of Plasmonic Photothermal Therapy (PPTT) in combating cancer. **M.R. Ali**, M.A. El-Sayed

10:40 COLL **599.** Assembly of ring-like nanostructure arrays via drop evaporation method. **Y. Bao**, N. Scherer, T. Witten

11:00 COLL **600.** Photo-oxidative degradation of single giant quantum dots. **N. Orfield**, S. Majumder, J.R. McBride, J.A. Hollingsworth, H. Htoon

11:20 COLL **601.** Highly sensitive surface-enhanced Raman scattering substrate of Ag thin film fabricated by gas-timing RF magnetron sputtering. **C. Sapcharoenkun**, A. Klamcheun, A. Treetong, P. Kasamechonchung, T. Wutikhun, P. Ukahapunyakul

11:40 COLL **602.** ALD-protected polyoxometalate water oxidation catalysts immobilized on light-absorbing metal oxide thin films for enhanced durability and photocurrent density. **S.M. Lauinger**, B. Piercy, W. Li, M.D. Losego, D. Wang, C.L. Hill

Section J

Moscone Center

2007

ACS Award in Colloid Chemistry: Symposium in honor of Nicholas A. Kotov

P. Podsiadlo, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 COLL **603.** Nanoparticles' interactions with viruses. **F. Stellacci**

9:05 COLL **604.** Nanoscale metal-organic frameworks: Emerging materials for catalysis. **Z. Tang**

9:35 COLL **605.** Molecular mechanisms in formation of metal oxide colloids in sol-gel processes. **V. Kessler**, G. Seisenbaeva

10:05 Intermission.

10:15 COLL **606.** Toward the self-assembly of layered multi-nano-composite films with complex anisotropies. R. Blell, M. Rémi, H. Hu, S. Bharani, V. Lemaire, M. Pauly, O. Félix, **G. Decher**

10:45 COLL **607.** Surface enhanced Raman scattering on cuprous oxide nanomaterials. **C. Jiang**

11:15 COLL **608.** Seeded growth and chemical transformations in metal nanoparticles. **L. Liz Marzan**

11:45 Concluding Remarks.

Mineral-Water Interface Chemistry

Sponsored by GEOC, Cosponsored by COLL and ENVR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Molecular & Bio-Inspired Photocatalysts

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Functional Lignocellulosics & Nanotechnology

Tuning Interfacial Phenomena with Ligno-Nanocellulosic Materials

Sponsored by CELL, Cosponsored by CARB and COLL

Elucidation of Mechanisms & Kinetics on Surfaces

Electrons

Sponsored by CATL, Cosponsored by COLL and ENVR

TUESDAY AFTERNOON

Section A

Moscone Center

2002

ACS Award Lectures

Cosponsored by CATL and WCC

R. Nagarajan, *Organizer*

H. Fairbrother, *Presiding*

2:00 Introduction of Awardee.

2:05 COLL **609. Award Address** (ACS Award in Colloid Chemistry sponsored by Colgate-Palmolive Company). Self-assembly of nanoparticles. **N. Kotov**

2:50 Introduction of Awardee.

‡ *Cooperative Cosponsorship*

2:55 COLL **610. Award Address** (ACS Award in Surface Chemistry sponsored by the ACS Division of Colloid & Surface Chemistry). Understanding of selective oxidation catalysis through surface science. **C.M. Friend**

3:40 Introduction of Awardee.

3:45 COLL **611. Award Address** (ACS Award for Research at an Undergraduate Institution sponsored by Research Corporation for Science Advancement). From nanogravimetry, photovoltaics, and plasmonics to elastic light scattering and Raman spectroscopy for theranostics and environmental remediation. **M.R. Hepel**

4:30 Introduction of Awardee.

4:35 COLL **612.** Nano Letters Award Lecture: Cool chemical transformations and hot carrier upconversion: Emerging plasmonic methods to improve renewable energy technologies. **J. Dionne**

Section B

Moscone Center

2004

Deposition & Etching of Nanostructures

Cosponsored by INOR

H. Fairbrother, L. McElwee-White, *Organizers*

A. V. Walker, *Organizer, Presiding*

2:00 COLL **613.** Cage molecule self-assembly. **P.S. Weiss**

2:30 COLL **614.** Development of photo-activated iodo-ene reaction for molecular layer deposition. **M. Lillethorup**, D.S. Bergsman, S.F. Bent

2:50 Intermission.

3:05 COLL **615.** Perfluoropentacene films on gold surfaces grown by supersonic molecular beam deposition. A. Yavuz, N. Sohrabnia, G. Bracco, **M. Danisman**

3:25 COLL **616.** Patterning diverse metallic materials directly from solution using laser thermal voxels. L.D. Zarzar, B. Swartzentruber, B. Donovan, P. Hopkins, **B. Kaehr**

3:45 COLL **617.** Hybrid Monte Carlo and continuum modeling of electron-beam induced processes using liquid reactants. **T.T. Hastings**, S. Esfandiarpour, E. Cao, S. Lami

Mineral-Water Interface Chemistry

Sponsored by GEOC, Cosponsored by COLL and ENVR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Novel Photocatalytic & Photoelectrode Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Functional Lignocellulosics & Nanotechnology

Dispersions, Gels, Foams, Colloids & Films

Sponsored by CELL, Cosponsored by CARB and COLL

Elucidation of Mechanisms & Kinetics on Surfaces

Organic Oxygenates

Sponsored by CATL, Cosponsored by COLL and ENVR

WEDNESDAY MORNING

Section A

Moscone Center

2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, S. Muralidharan, A. N. Parikh, N. Srividya, *Organizers*

M. Nieh, *Organizer, Presiding*

J. Nickels, *Presiding*

8:30 COLL **618.** Examining cell migration and cell junction dynamics using polymer gel-supported lipid bilayers. **K.D. Shilts**, Y. Ge, C. Naumann

8:50 COLL **619.** Artificial biomembrane microsystems for highly sensitive analysis of membrane proteins. **R. Watanabe**

9:15 COLL **620.** Synthesis and characterization of supported lipid bilayer membranes from complex lipid mixtures. G. Hardy, J. Shapter, M. Alam, **S. Zauscher**

9:40 COLL **621.** Modulation of lipid membrane structure and dynamics in the presence of amyloid-ß peptide. **T. Hauß**, M.A. Barrett, N.A. Dencher

10:05 COLL **622.** Probing membrane protein organization and dynamics in planar model membranes using single molecule-sensitive confocal detection techniques. **C. Naumann**, Y. Ge, K. Shilts

10:30 COLL **623.** Fusion processes of proteoliposomes into supported planar lipid bilayers. **R. Tero**, K. Fukumoto, M. Yoshida, A. Hirano-Iwata, M. Niwano

10:55 COLL **624.** Topographic control of membrane functions. **R. Ashkar**, M. Zhernenkov, R.G. Toomey, R. Pynn, J. Katsaras, J. Carrillo, B. Sumpter

11:20 COLL **625.** Tubule formation and retraction in the interaction of supported lipid bilayers with SDS. E.J. Eis, J. Churchwell, M. Staykova, **C.D. Bain**

11:45 COLL **626.** Interfacial structure of water confined between phospholipid-coated surfaces probed by infrared-visible Sum Frequency Generation (SFG) spectroscopy. N. Dhopatkar, X. Shi, J. Brown, X. Li, A.W. Smith, **A.N. Dhinojwala**

Section B

Moscone Center

2004

Colloidal Nanoparticle Synthesis & Assembly

Synthesis & Growth

Y. Sun, S. Wu, *Organizers*

H. Fan, H. Htoon, *Organizers*, *Presiding*

8:30 COLL **627.** In situ study of colloidal nanoparticle growth and assembly. **H. Zheng**

9:00 COLL **628.** Polymer-assisted deposition: A simple process for a wider range of electronic materials. **Q. Jia**

9:30 COLL **629.** *In situ* Variable-Temperature Liquid Cell Transmission Electron Microscopy (VT-LCTEM) study of size-stabilized Covalent Organic Framework (COF) nanoparticle nucleation and growth during solvothermal synthesis. **L.R. Parent**, B.J. Smith, C. Park, W.R. Dichtel, N.C. Gianneschi

9:50 COLL **630.** Paramagnetically amplified optical activity of chiral nanoparticles. **J. Yeom**, A. Farias de Moura, N. Kotov

10:10 COLL **631.** Photoluminescence blinking and polarization anisotropy of single colloidal semiconductor nanoplatelets. **Z. Hu**, A. Singh, J.A. Hollingsworth, H. Htoon

10:30 COLL **632.** Migration and structural evolution of carbon-encapsulated Fe nanoparticles via *in situ* TEM. **R.V. Grieshaber**, Z. Liu, J. Yang

10:50 COLL **633.** Two-phase synthesis of metal sulfide nanoparticles. **L. Bian**, J. Maier, S. Marra, K. Ring, P. Goulet

11:10 COLL **634.** Multi-shelled metal oxides hollow microspheres: Synthesis and applications. **D. Wang**, J. Wang, R. Yu, H. Zhao

11:40 COLL **635.** Effect of ligand asymmetry in the properties of nanoparticle membrane. **X. Lin**, Z. Jiang, J. Wang, S. Deshmukh, P. Kanjanaboos, G. Kamath, Y. Wang, H. Chan, B. Narayanan, S. Sankaranarayanan, H. Jaeger

Section C

Moscone Center

2006

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Technique Development in Interfacial Science

Cosponsored by CATL

S. H. Kim, R. M. Rioux, *Organizers*, *Presiding*

8:30 COLL **636.** High-energy-resolution x-ray absorption spectroscopy: A powerful method to push the frontiers of in-situ x-ray absorption spectroscopy of catalysts. **S.R. Bare**, D. Sokaras, T. Kroll, A. Gallo, A.S. Hoffman, B.C. Gates

9:00 COLL **637.** Degree of rate control: A tool for analyzing microkinetic models and high-throughput computational screening of catalyst materials. **C.T. Campbell**, Z. Mao

9:30 COLL **638.** High spatial resolution mapping of catalytic reactions on single nanoparticles. **E. Gross**

10:00 COLL **639.** Monitoring real-time dynamics of nanoparticle formation via trading space with time strategy and synchrotron x-ray absorption spectroscopy technique. S. Bakhti, N. Destouches, M. Ahmed, **S. Alayoglu**

10:30 COLL **640.** Time-resolved characterization of hierarchical diffusion and reactions in acidic zeolites and zeotypes with Temporal Analysis of Products (TAP) experiments. E. Redekop, J. Martinez, M. Morten, B.T. Bleken, R. Fushimi, M. Mykland, **U. Olsbye**

11:00 COLL **641.** Solution calorimetry methods for the study of catalytic solid-liquid interfaces. **R.M. Rioux**

Section D

Moscone Center

2008

Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment

A. H. Flood, *Organizer*

S. L. Tait, *Organizer, Presiding*

8:30 COLL **642.** Tuning the physical properties of MoS_2 membranes through organophosphonate-based surface functionalization. S. Schwarzwälder, R. Csiki, S. Zhao, K. Larsson, J. Schwartz, M. Stutzmann, U. Wurstbauer, **A. Cattani-Scholz**

8:50 COLL **643.** Bottom-up hierarchical self-assembly of zwitterionic dendrimers into stimuli responsive dynamic nanotubes. **S. Eghtesadi**, M. Kashfipour, X. Sun, S. Lillard, T. Liu

9:10 COLL **644.** 2D phase evolution and solvation in dimethyl formamide-lithium ethylene dicarbonate films on Ag(111). **J.E. Reutt-Robey**

9:40 COLL **645.** Functionalization of 2D materials: The molecular approach. **S. De Feyter**

10:10 COLL **646.** Supramolecular arrays and heterostructures on hexagonal boron nitride. **P. Beton**, V. Korolokov, J. Kerfoot, M. Baldoni, N. Besley, E. Besley, N.R. Champness, L. Yang, T. Taniguchi, K. Watanabe

10:40 COLL **647.** Self-assembly and post-assembly chemical transformation of reactive compositionally patterned monolayers. **M. Zimmt**, C. Fang, J. He, R.A. Shelp, Y. Yang

11:10 COLL **648.** Hierarchy in the self-assembly of novel chiral dyes for photovoltaic applications. **D. Amabilino**, F. Pop

11:40 COLL **649.** Structure and function of bilayer organic photovoltaics. **M.E. Thompson**

Section E

Moscone Center

2010

Basic Research in Colloids, Surfactants & Nanomaterials

Biomolecular Systems

R. Nagarajan, *Organizer*

K. S. Raja, *Presiding*

8:30 COLL **650.** Biophysical properties of salt-induced simple coacervation of interfacial mussel adhesive proteins. **B. Yang**, H.J. Cha

8:50 COLL **651.** Effect of additives on the crystal morphology of amino acids: A theoretical and experimental study. **E. Constance**, M. Mohammed, K. Aslan

9:10 COLL **652.** Adsorption behaviors of mussel proteins on biomaterials with different surface chemistries: A fundamental understanding of mussel inspired adhesive designs. **Y. Wei**, C. Lin, Y. Lai, Y. Tang, P. Wang, D. Li, Y. Huang

9:30 COLL **653.** Sponge mimetic tubules: Programmable stigmergy scaffolds for 3D marine, mammalian cell culture and bioelectronics. **K.S. Raja**, K. Punia

9:50 COLL 654. Dynamic interactions of amelogenin with hydroxyapatite surfaces are dependent on protein phosphorylation and solution pH. **A.E. Gerdon**, C.P. Connelly, T. Cicuto, J.D. Leavitt, A. Petty, A. Litman, H. Margolis

10:10 COLL 655. Investigation of oligomerization of amyloidogenic peptides at nanoscale gold colloidal interface. **K. Yokoyama**

10:30 COLL 656. Hydrodynamic effects in concentrated protein solutions with repulsive and attractive interactions. **D. Corbett**, P.J. Davis, C. van der Walle, S. Uddin, A. Pluen, R. Curtis

10:50 COLL 657. Effects of macromolecular crowding on a coacervation-based model for intracellular organization. **A. Marianelli**, B. Miller, C.D. Keating

11:10 COLL 658. Effects of phosphatidylcholine vesicles on adsorption kinetics at an air-water interface. **J. Staton**, S.R. Dungan

11:30 COLL 659. New colloidal approaches for human norovirus cleanup and deactivation using surfactants and copper-ion based disinfectants. **B. Mertens**, M. Moore, L. Jaykus, O.D. Velev

11:50 COLL 660. Spin selectivity in DNA-mediated charge transport: Base sequence and structure relationships. **J. Abendroth**, N. Nakatsuka, M. Ye, D. Kim, E. Fullerton, A.M. Andrews, P.S. Weiss

Section F

Moscone Center

2012

Applied Biosensing Based on Functional Colloids

R. Alvarez Puebla, L. Liz Marzan, W. Parak, J. Sagalés, G. F. Strouse, *Organizers*

N. Feliu, *Presiding*

8:30 COLL 661. Connecting the triangle. **J. Sagalés**

8:50 COLL 662. Optical visualization and quantification of enzyme activity using dynamic droplet lenses. **L.D. Zarzar**, J. Kalow, X. He, J. Walish, T.M. Swager

9:10 COLL 663. Sandwich immunoassays for infectious disease diagnstics using noble metal nanoparticles. C. Yen, H. de Puig, J.O. Tam, M. Sanchez, M. Carre, J. Gomez-Marquez, I. Bosch, L. Gehrke, **K. Hamad-Schifferli**

9:40 COLL 664. Measuring heparin activity with a nanoparticle-functionalized catheter. J. Wang, F. Chen, **J.V. Jokerst**

10:10 COLL 665. Highly quenching nickel-gold core-shell magnetic plasmonic nanoparticles for biosensing. **P.N. Vakil**, G.F. Strouse

10:30 COLL 666. Enhanced energy coupling within a nanometal plasmon field for molecular ruler and in-vitro event mapping technologies. **G.F. Strouse**

Section G

Moscone Center

2001

Chemistry & Physics of Tribology

Biotribology, Biomimetic Systems & Lubrication in Aqueous Media

F. Mangolini, M. Ruths, *Organizers*

B. Krick, J. Wong, *Presiding*

8:30 COLL 667. Updating the mechanics of cartilage and joint lubrication. **D. Burris**

9:05 COLL 668. Colloid-probe AFM on gels and humidity-dependent AFM on hydrophilic networks: Aqueous tribology and glass-rubber transitions. **G.D. Haugstad**

9:25 COLL 669. Nanotribological studies of polymer brushes fabricated by near-field and interferometric lithography. Z. Zhang, O. Al Jaf, S.P. Armes, **G.J. Leggett**

9:45 COLL 670. Wear protection without surface modification: Is it possible? **X. Banquy**, J. Faivre, B. Shrestha, J. Burdynska, G. Xie, F. Moldovan, L. David, T. Delair, S. Benayoun, K. Matyjaszewski

10:05 COLL 671. Effect of multivalent counterions to the structure and lubrication properties of polystyrene sulfonate brushes. **J. Yu**, M.V. Tirrell

10:25 COLL 672. Tactile and hair–hair friction behavior of hair fibers. **N. Nordgren**, L. Skedung, N. Baghdadli, M.W. Rutland, G.S. Luengo

10:45 COLL 673. Effects of 3D surface patterning on the tribology of human stratum corneum and the topology of a polyurethane skin surface model. R. Jin, I. Liao, X. Xu, C. Cazeneuve, J.C. Chang, J. Langer, **M. Ruths**, G.S. Luengo

Section H

Moscone Center

2003

Basic Research in Colloids, Surfactants & Nanomaterials

Nanomedicine

R. Nagarajan, *Organizer*

K. Slowinska, *Presiding*

8:30 COLL 674. Harnessing shape and bi-specific antibodies for improved cell-targeting efficiency of poly(ethylene glycol) capsules. **D. Song**, J. Cui, Y. Ju, H. Sun, K. Thurecht, F. Caruso

8:50 COLL 675. Galectin-1-based tumor-targeting for gold nanostructure mediated theranostics. **S.V. Jenkins**, D. Nedosekin, R. Dings, J. Chen, R. Griffin

9:10 COLL 676. Stem cell/nanoparticle conjugates for targeted cancer therapy. **J.M. Berlin**

9:30 COLL 677. Thermo-responsive hybrid peptide nanoparticles in targeting-free cell selection and uptake. **K. Slowinska**

9:50 COLL 678. Screening of prostate cancer cells using Zn(II) sensing SERS nanoprobe. **P.C. Ray**

10:10 COLL 679. Drug delivery using layered structured nanomaterials. **J.L. Colon**, J. Gonzalez, Y. Kan, V. Bakhmoutov, A. Clearfield

10:30 COLL 680. Probing the stability of liposomal spherical nucleic acids for therapeutic design. **B. Meckes**, R. Banga, C.A. Mirkin

10:50 COLL 681. Development and characterization of free-standing nano films loaded with iron nanoparticles for magnetic drug targeting. **M. Sakuragi**, H. Murayama, K. Taguchi, K. Kusakabe

11:10 COLL 682. Synthesis and biomedical application of metal and metaloxide nanocrystals. **Q. Zhang**, S. Tong, Y. Hu, G. Bao, **V. Colvin**

11:30 COLL 683. Nanolipoprotein particles for delivery of theraputics to the brain. **S.F. Gilmore**, N.A. Be, H.A. Enright, M.A. Malfatti, A. Rasley, J. Osburn, S. Peters, N.O. Fischer

11:50 COLL 684. Formulation and study of highly stable, semifluorinated nanoemulsions with theranostic applications. **A.R. Barres**, S. Mecozzi

Section I

Moscone Center

2005

Basic Research in Colloids, Surfactants & Nanomaterials

Polymer Materials & Gels

R. Nagarajan, *Organizer*

T. J. McCarthy, *Presiding*

8:30 COLL 685. Ice adhesion reducing polymers and prepolymers based on siloxanes and F-POSS. **R. Simons**, S. Li, L. Russel, S. Bateman, J. Seebergh, D. Berry

8:50 COLL 686. Withdrawn.

9:10 COLL 687. Rediscovering silicones: Water repellency and water permeability. P. Bian, **T.J. McCarthy**

9:30 COLL 688. Development of new multi-functional polycarbonate platforms. **N. Park**, J. Hedrick

9:50 COLL 689. Withdrawn.

10:10 COLL 690. Directly linear alignment as different deacetylation of chitosan under electric field. **Y. Chun**, Y. Ko, T. Do, U. Choi

10:30 COLL 691. Stimuli-responsive cyclodextrin-modified microgels: Functional carriers with dynamic crosslinks and binding domains. **A. Pich**, D. Schmitz

10:50 COLL 692. Shape stability and mechanical properties of rhombic dodecahedron multilayer hydrogel capsules at various pH. **N. Gupta**, J. Chen, V.A. Kozlovskaya, B. Xue, E.P. Kharlampieva

11:10 COLL 693. Synthesis of monolithic $Cu_2(OH)_3Br$ aerogels. **T.M. Fears**, J.D. Colvin, S.O. Kucheyev

11:30 COLL 694. Synthesis of poly (2-methoxyethyl acrylate)-based hydrogel particles for bio-coatings and carriers. **T. Kureha**, D. Suzuki

11:50 COLL 695. Gelation of vegetable and mineral oils by an efficient and versatile low-molecular-mass gelator. **D. Bajani**, J. Dey

Bio-based Gels & Porous Materials

Biopolymer Hydrogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Deposition & Etching of Nanostructures

Sponsored by INOR, Cosponsored by COLL‡

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

Sponsored by GEOC, Cosponsored by COLL, ENVR and NUCL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Spectroscopy & Microscopy of Photocatalytic & PEC Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Chemical Principles of Environmental, Cellular & Organismal Nanotoxicology

Sponsored by ENVR, Cosponsored by COLL

Mineral-Water Interface Chemistry

Sponsored by GEOC, Cosponsored by COLL and ENVR

Functional Lignocellulosics & Nanotechnology

Dispersions, Gels, Foams, Colloids & Films

Sponsored by CELL, Cosponsored by CARB and COLL

Elucidation of Mechanisms & Kinetics on Surfaces

Organic Oxygenates

Sponsored by CATL, Cosponsored by COLL and ENVR

WEDNESDAY AFTERNOON

Section A

Moscone Center

2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

S. Muralidharan, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

J. Katsaras, *Organizer, Presiding*

R. Ashkar, *Presiding*

2:00 COLL 696. Preparation, characterization, and application of nanopore-supported phospholipid bilayers. **D. Bryce**, J.P. Kitt, J.M. Harris

2:20 COLL 697. Biomimetic construction of phospholipid membranes. **R.J. Brea Fernández**, C.M. Cole, A.K. Rudd, N.K. Devaraj

2:45 COLL 698. Interplay of structure and dynamics in mixed lipid bilayers. **E.G. Kelley**, R. Ashkar, R. Bradbury, P. Butler, M. Nagao

3:10 COLL 699. Neutron scattering to study membrane systems: From lipid vesicles to living cells. **J. Nickels**, S. Chatterjee, C.B. Stanley, S. Qian, X. Cheng, D. Myles, R.F. Standaert, J. Elkins, J. Katsaras

3:35 COLL 700. Human lipoproteins at model cell membranes: Role of the lipoprotein class on lipid dynamics. **K. Browning**, T. Lind, S. Maric, S. Malekkhaiat-Häffner, G.N. Fredrikson, E. Bengtsson, M. Malmsten, M. Cárdenas

4:00 COLL 701. Lipoprotein structure dependency on lipid cargo and exchange dynamics: Implications for atherosclerosis development. **S. Maric**, T. Lind, J. Lyngsø, E. Bengtsson, G.N. Fredrikson, M. Moulin, M. Haertlein, T. Forsyth, J. Pedersen, M. Cardenas

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4:25 COLL 702. Probing the structure and dynamics of proteins using neutron scattering. **M. Sharp**

4:50 COLL 703. Effect of cholesterol on the elastic and viscous properties of dimyristoylphosphatidylcholine bilayers. **R. Bradbury**, M. Nagao, E.G. Kelley

Section B

Moscone Center

2004

Colloidal Nanoparticle Synthesis & Assembly

Y. Sun, S. Wu, *Organizers*

H. Fan, H. Htoon, *Organizers*, *Presiding*

2:00 COLL 704. Observation of nucleation and growth during the formation of cadmium selenide and iron oxide nanoparticles and their use for biomedical imaging. **H. Weller**

2:30 COLL 705. Suppressed-blinking green-emitting giant quantum dots: From synthesis to structure to function. **J.A. Hollingsworth**, N. Mishra, N. Orfield, J.R. McBride, C. Hanson, S. Click, Z. Hu, H. Htoon

3:00 COLL 706. Tunable quasi-amorphous photonic materials with pigmentary colloidal nanostructures. **J. Han**, E. Lee, J. Dudoff, M. Bagge-Hansen, J.R. Lee, A.J. Pascall, J.D. Kuntz, T. Willey, M.A. Worsley, Y.J. Han

3:20 COLL 707. Chemical intercalation of superatomic solids. **E. O'Brien**, X. Roy

3:40 COLL 708. Self-assembly of nanoparticles via co-crystallization with proteins. **H. Kim**, V. Colvin

4:00 COLL 709. Reversible and precise self-assembly of Janus metal-organosilica nanoparticles through a linker-free approach. **H. Hu**, Q. Zhang

4:20 COLL 710. New class of branched and nanofibrous dendrimeric polymer particles with extraordinary adhesive and structure-building capabilities. **S. Roh**, S.D. Stoyanov, O.D. Velev

4:40 COLL 711. Controlling size in nanoparticle syntheses using the extended LaMer mechanism. **D. Huber**

5:10 COLL 712. Colloidal superparticles from colloidal crystallization in closed systems. **Y.C. Cao**

Section C

Moscone Center

2006

Molecular Surface Science, Nanomaterials & Catalysis: Symposium in honor of Gabor Somorjai at 80

Electrons & Photons in Interfacial Science

Cosponsored by CATL

S. H. Kim, R. M. Rioux, *Organizers*, *Presiding*

2:00 COLL 713. Surface bonding and chemistry for pyridine-catalyzed CO_2 reduction on GaP. **B.E. Koel**

2:30 COLL 714. Intercalation of metal ions into the interlayer region of layered manganese oxide for improved water oxidation electrocatalysis. **D.R. Strongin**, A.C. Thenuwara, S. Shumlas, I.G. McKendry, R.C. Remsing, M. Zdilla, Q. Kang, M.L. Klein, E. Borguet, N. Attanayake, J. Sun, L. Frazer

3:00 COLL 715. Understanding the surface reactions of the lithium-air battery and its consideration for usage in an automotive application. **C.J. Brooks**, Q. Xu, E. Kreidler

3:30 COLL 716. Experimental and computation studies of the reaction of hydrogen and organic peroxide on molybdenum hydrogen bronze surfaces. **N.F. Materer**, A.W. Apblett

4:00 COLL 717. Systematic approaches to modify the surface and electronic structure of TiO_2 nanocrystals. C. Balasanthiran, S. Varapragasam, S. Mia, R.M. Rioux, **J.D. Hoefelmeyer**

4:30 COLL 718. Photoelectrical response of mesoporous metal oxides decorated with size controlled platinum nanoparticles under argon and oxygen gas. A. Sapi, A. Kukovecz, **Z. Konya**

Section D

Moscone Center

2008

Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment

S. L. Tait, *Organizer*

A. H. Flood, *Organizer, Presiding*

2:00 COLL 719. 4D nanolithography using a flow-through polymer printer. **A.B. Braunschweig**

2:30 COLL 720. Colored soaps for photonics. **M. Presselt**, F. Herrmann-Westendorf, M. Kaufmann, S.K. Das, M.L. Hupfer, B. Dietzek

2:50 COLL 721. Metal-organic coordination chains at surfaces: Chemical activity of single-site transition metal centers. **S.L. Tait**, C. Tempas, L. Chen, T.W. Morris, C.G. Williams, M. Wang, D.L. Wisman, B.J. Cook, A.V. Polezhaev, K.G. Caulton

3:20 COLL 722. Computational design of metal-ligand coordination centers for catalytic applications. **T.S. Rahman**

3:50 COLL 723. Two-dimensional organic heterostructures and Co-crystals. **A. Enders**

4:20 COLL 724. Axial binding to supported metal porphyrins at the solution-solid interface. **K. Hipps**, U. Mazur Hipps

4:50 COLL 725. Development of fragment-based quantum chemical models for understanding supramolecular interactions and self-assembly. **K. Raghavachari**, A. Sengupta, S. Debnath

5:20 COLL 726. Tuning the exchange coupling of transition metal complexes to gold substrates by magnetic fields. **T. Pope**, K. Yang, H. Chen, L. Liu, D. Wang, L. Tao, W. Xiao, X. Fei, H. Luo, S. Du, T. Xiang, W. Hofer, H. Gao

5:40 COLL 727. Theoretical studies of adsorption and self-assembly of probe organic molecules at metal oxide surfaces. **X. Gong**, Y. Yu, Q. Cuan

Section E

Moscone Center

2010

Basic Research in Colloids, Surfactants & Nanomaterials

Bionanomaterials

R. Nagarajan, *Organizer*

P. Kral, *Presiding*

2:00 COLL 728. Enhanced immobilization of His-tagged enzymes using porous nickel silicate covered magnetic nanoparticles. **M. Shin**, B. Kang, N. Yoon, M. Kim, J. Ki, S. Han, J. Ahn, S. Haam

2:20 COLL 729. Diffusion of biomolecules in vesicle assembled RNA-based coacervates. **F. Pir-Cakmak**, W.M. Aumiller, B. Davis, C.D. Keating

2:40 COLL 730. Atomistic modeling of highly specific bio-active nanoparticles and micelles. **P. Kral**

3:10 COLL 731. Controlling colloidal drug aggregate stability and protein adsorption. **A. Ganesh**, J. Logie, C. McLaughlin, B. Shoichet, M.S. Shoichet

3:30 COLL 732. Investigation of silk fibroin thin films for the improvement of bioactive peptide-based biosensors. **L. Soblosky**, J.R. Uzarski

3:50 COLL 733. Oligonucleotide - peptide complexes: Phase control by hybridization. **J. Vieregg**, M.J. Lueckheide, A. Marciel, L. Leon, M.V. Tirrell

4:10 COLL 734. Ultra-rapid crystallization of L-alanine using monomode microwaves, indium tin oxide, and metal-assisted and microwave-accelerated evaporative crystallization. **C. Lansiquot**, Z. Boone-Kukoyi, R. Shortt, N. Thompson, H. Ajifa, B. Kioko, E. Constance, T. Clement, B. Ozturk, K. Aslan

4:30 COLL 735. Synthesis of platinum (II) – nuclear localization sequence peptide hybrid for nanoparticle development and anticancer therapy. M. Wlodarczyk, O. Camacho-Vanegas, S. Dragulska, A. Jarzecki, P.R. Dottino, J.A. Martignetti, **A.J. Mieszawska**

4:50 COLL 736. Design and evaluation of trigger-responsive DNA-drug nanostructures. **X. Tan**, X. Lu, F. Jia, X. Liu, Y. Sun, J. Logan, K. Zhang

5:10 COLL 737. Production of protein nanofibers using new timesaving methodologies for the design of innovative biomedical applications. **N.H. Silva**, T. Carvalho, A.A. Silvestre, I. Marrucho, C. Freire

Section F

Moscone Center

2012

Basic Research in Colloids, Surfactants & Nanomaterials

Carbon Materials

R. Nagarajan, *Organizer*

J. R. Uzarski, *Presiding*

2:00 COLL 738. Carbon nanotube-quantum dot nanohybrids: Coupling with single particle control in aqueous solution. **A. Attanzio**, M. Palma

2:20 COLL 739. Fabrication of laser-induced graphene under controlled gas atmosphere – from superhydrophilic to superhydrophobic. **Y. Li**, D. Luong, J. Zhang, J.M. Tour

2:40 COLL 740. Fabrication of carrageenan/carbon nanotubes conducting patterns by extrusion printing method. **A. Aldalbahi**, M. Panhuis, C. Fan

3:00 COLL 741. Multiplexed graphene-based nanomaterials for discriminatory sensing: A combined fundamental and applied experimental approach. **J.R. Uzarski**, E. Nallon, S. McGraw, M. Wiederoder, T. Lawton, C. Bright

3:30 COLL 742. Withdrawn.

3:50 COLL 743. Shear thickening behavior of graphene nanoplatelets and carbon nanotubes containing fumed silica suspensions. **M. Zabet**, K. Trinh, H. Toghiani, T. Lacy, C.U. Pittman, S. Kundu

4:10 COLL 744. Plasma-enhanced graphene and graphene oxide based conducting polymer composites for solar cell and biosensor applications. **A. Uygun Oksuz**, S. Cogal, G. Celik Cogal, S. Tunc, F. Kuralay, S. Erten Ela, M. Omastova, S. Ahmad

4:30 COLL 745. Synthesis and characterization of water-based dispersions of high-purity, thin graphene oxide sheets from different graphitic sources. **D. Jasim**, K. Kostarelos

4:50 COLL 746. Bioinspired Polydopamine (PDA) chemistry meets Ordered Mesoporous Carbons (OMCs): A benign surface modification strategy for versatile functionalization. **Y. Song**, G. Ye, J. Wang, K. Matyjaszewski

Section G

Moscone Center

2001

Chemistry & Physics of Tribology

Tribology in Extreme Environments & Advances in Solid Lubrication

F. Mangolini, M. Ruths, *Organizers*

X. Banquy, S. Didziulis, *Presiding*

2:00 COLL 747. Aging effects on the transient frictional behavior of MoS_2-based solid lubricants for use in extreme environments. **M. Dugger**

2:35 COLL 748. Understanding friction in MoS_2: Structure, oxidation and run-in. J. Curry, M. Sidebottom, H. Luftman, N. Strandwitz, N. Argibay, **B. Krick**

2:55 COLL 749. Lubricant effects in space system performance. **S.V. Didziulis**, P.P. Frantz, V. Oklejas, J.M. Helt

3:15 COLL 750. Interactions between oil-soluble phosphonium-phosphate ionic liquids and steel in the mixed and boundary lubrication regime. **S. Berkebile**, N. Murthy, J. Mogonye

3:35 COLL 751. Linking microstructure to wear-induced pitting corrosion in aged 2507 super duplex stainless steel. **J.M. Shockley**, D. Horton, K.J. Wahl

3:55 COLL 752. Amazing friction properties of graphene and water. **M. Salmeron**, J. Park

4:30 COLL 753. Effect of thickness and chemical reduction of graphene oxide on nanoscale friction. **J. Park**, S. Kwon, H. Lee

4:50 COLL 754. Studies of the dynamic frictional properties of 2D nanomaterials. M.B. Elinski, Z. Liu, M. Negrito, **J.D. Batteas**

5:10 COLL 755. Boron nitride nanomesh model system for stiction and adhesion. **S. Mertens**, A. Hemmi, S. Muff, O. Groening, S. De Feyter, J. Osterwalder, T. Greber

5:30 COLL 756. Understanding the influence of environment and surface patterning on the tribological behaviour of silicon-oxide containing diamond-like carbon (a-C:H:Si:O) films. **K. Koshigan**, J. Lengaigne, R. Carpick, J. Fontaine, J. Sapieha, L. Martinu

Section H

Moscone Center

2003

Basic Research in Colloids, Surfactants & Nanomaterials

Nanomedicine

R. Nagarajan, *Organizer*

M. Ruths, *Presiding*

2:00 COLL 757. Antioxidant carbon nanomaterials for treating autoimmune disorders. **L.G. Nilewski**, R. Huq, E.L. Samuel, W.K. Sikkema, R. Pautler, D.B. Corry, C. Beeton, J.M. Tour

2:20 COLL 758. Characterization of amphiphilic copolymer micelles for drug delivery. X. Xu, B. Gupta, S. Kaur, J. Nguyen, R. Jin, A.C. Watterson, **M. Ruths**

2:40 COLL 759. Tuning the drug uptake and release from silica nanostructures as a function of etching medium. H. Thawani, V. Patel, S. Singh, **A. Karakoti**

3:00 COLL 760. Filomicelles deliver retinoids and chemotherapeutics to durably control carcinoma cell fate. **P. Nair**, D.E. Discher

3:20 COLL 761. Influences of serum proteins on the uptake of Fe_3O_4 nanoparticles by human breast cancer cells. **L. Guo**, T. Wang, N. He

3:40 COLL 762. Hyperthermia properties of superparamagnetic ferrite (MFe_2O_4) nanoparticles synthesized via the thermal decomposition method. **S. Sabale**, V. Jadhav, X. Yu

4:00 COLL 763. Microwave heating of synthetic skin for potential treatment of gout using the metal-assisted and microwave-accelerated decrystallization technique. **S. Toker**, Z. Boone-Kukoyi, N. Thompson, H. Ajifa, T. Clement, B. Ozturk, K. Aslan

4:20 COLL 764. Novel platelet-repellent polyphenolic surfaces and their micropattern for platelet adhesion detection. **L. Yang**, L. Han, L. Jia

4:40 COLL 765. Modeling of polymer based micelles and DNA delivery medicines. **Y. Han**, P. Kral

5:00 COLL 766. Surface modification of nanoscale diamond for biolabelling with the nitrogen vacancy center. P. Tran, P.J. Sandoval, J. Hnatek, E.S. Favre, A. Arreola, A.A. Len, I. Laaguidi, A. Hernandez, D. Nordlund, **A. Wolcott**

5:20 COLL 767. Classification of bacteria by surface enhanced Raman spectroscopy and principal component analysis. **S.J. Jones**, S.S. Sinha, P.C. Ray

Section I

Moscone Center

2005

Basic Research in Colloids, Surfactants & Nanomaterials

Colloidal Assembly

R. Nagarajan, *Organizer*

S. A. Santer, *Presiding*

2:00 COLL 768. Light driven diffusioosmosis: Manipulation of particle assembly. **S.A. Santer**

2:20 COLL 769. Block copolymer morphology switch *via* colloidal assembly and local reorganization. **D. Wright**, J.P. Patterson, M. Touve, A. Carlini, N.C. Gianneschi

2:40 COLL 770. Tailored nanoparticles by wet chemical particle technology: From lab to pilot scale. **K. Mandel**

3:00 COLL 771. Multipole re-expansion model for assembly of dielectric particles in external electric field. **G. Goel**, A. Nayeer, A. Ranjak, S. Gupta

3:20 COLL 772. Patchy particles via cluster fusion. **Z. Gong**, T. Hueckel, G. Yi, S. Sacanna

3:40 COLL 773. Modeling of magnetization in self-assembled magnetic nanocubes. **C. Wang**

4:00 COLL 774. Reconfigurable colloids via stimulated dewetting. **M. Youssef**, T. Hueckel, G. Yi, S. Sacanna

4:20 COLL 775. Burstable nanostructured micro-raspberries: Toward redispersible, adjustable nanoparticles from dry powders. **C. Stauch**, T. Ballweg, R. Luxenhofer, K. Mandel

4:40 COLL 776. Inducing an order-order morphological transition via chemical degradation of amphiphilic diblock copolymer nano-objects. **L.P. Ratcliffe**, C. Couchon, S.P. Armes, J.M. Paulusse

Bio-based Gels & Porous Materials

Biopolymer Organogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Deposition & Etching of Nanostructures

Sponsored by INOR, Cosponsored by COLL‡

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

Sponsored by GEOC, Cosponsored by COLL, ENVR and NUCL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Devices, Assemblies & Hybrid Processes

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Functional Lignocellulosics & Nanotechnology

Responsive Materials & Biosensors

Sponsored by CELL, Cosponsored by CARB and COLL

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms: Hydrogenation

Sponsored by CATL, Cosponsored by COLL and ENVR

WEDNESDAY EVENING

Chemical Principles of Environmental, Cellular & Organismal Nanotoxicology

Sponsored by ENVR, Cosponsored by COLL

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Sponsored by GEOC, Cosponsored by COLL and ENVR

General Session

Sponsored by GEOC, Cosponsored by COLL and ENVR

THURSDAY MORNING

Section A

Moscone Center

2002

Biomembrane Synthesis, Structure, Mechanics & Dynamics

J. Katsaras, M. Nieh, A. N. Parikh, N. Srividya, *Organizers*

S. Muralidharan, *Organizer, Presiding*

9:00 COLL 777. Controlled drug release from magneto-liposomes via ultrasound generation. **G. Podaru**, V. Chikan, P. Prakash

9:20 COLL 778. Mechanical characterization of self-assembled surfactant micelles at graphite surfaces via atomic force microscopy. **B.L. Micklavzina**, M.L. Longo, S. Zhang, H. He

9:40 COLL 779. Carbon nanotube enhancement of water and ion permeability of diblock copolymer membranes. **J. Sanborn**, R. Tunuguntla, X. Chen, A.N. Parikh, A. Noy

10:00 COLL 780. Shape morphogenesis in giant lipid vesicles in an osmotic field gradient. **S. Hong**, V. Sharma, V. Nguyen, D. Gettel, J. Sanborn, A.N. Parikh

10:20 COLL 781. Single-molecule detection of biomarker molecules in a nanometric gap structure with fluid lipid membrane. **K. Ando**

10:40 COLL 782. Phase separation and curvature generation in biphasic giant lipid vesicles reconstituting plant plasma membrane lipids. **S. Emami**, V. Ngassam, A.N. Parikh

11:00 COLL 783. Evaluating the interactions of lipid raft and proteins involved in phototransduction by using a micropatterned model membrane. **Y. Tanimoto**

11:20 COLL 784. Morphological consequences of surface-mediated spinodal decomposition inside giant vesicles. **W. Su**, D. Gettel, M. Chabanon, S. Hong, P. Rangamani, A.N. Parikh

11:40 COLL 785. Small molecule induced fusion of a model protocell membrane composed of fatty acids: A new insight into the membrane fusion monitored through fluorescence lifetime imaging microscopy. **N. Kundu**, N. Sarkar

Section B

Moscone Center

2004

Colloidal Nanoparticle Synthesis & Assembly

H. Fan, H. Htoon, Y. Sun, S. Wu, *Organizers*

F. Bai, Y. Jiang, *Presiding*

8:30 COLL 786. Modeling nanoparticle assembly: Using polymer coatings, interfaces, and pressure to build 1D, 2D, and 3D nanostructures. **J.M. Lane**

9:00 COLL 787. Constructing theranostics based on fluorecent carbon nanodots. **Z. Sun**

9:30 COLL 788. Engineering bimetallic nanocrystals as artificial enzymes for colorimetric detection of disease biomarkers. **X. Xia**, H. Ye

10:00 COLL 789. Tuning functional nanoparticulate and nanoporous structures using atomic layer deposition. **Y. Jiang**

10:20 COLL 790. Atomistic modeling of nanoparticle formation, modification and self-assembly in liquid cells. **P. Kral**

10:40 COLL 791. Modeling of self-assembly dynamics of charged nanoparticles in liquid cells. **F. Sanoj**

11:00 COLL 792. Modeling the nucleation and growth of palladium nanoparticles in the presence of capping ligands. **S. Mozaffari**, W. Li, C. Thompson, A.M. Karim

11:20 COLL 793. Cellulose nanocrystal-derived stimulus-responsive cholesteric microgels having catalytic properties. **S. Cho**, Y. Li, M. Seo, E. Kumacheva

11:40 COLL 794. Controlled self-assembly of porphyrin and applications. **F. Bai**

Section C

Moscone Center

2006

Basic Research in Colloids, Surfactants & Nanomaterials

Surface Studies

R. Nagarajan, *Organizer*

T. Lawton, *Presiding*

8:30 COLL 795. Probing heterogeneity and bonding at silica surfaces through single-molecule investigation of base-mediated linkage failure. **K. Lupo**, D. Hinton, J. Ng, N. Padilla, R.H. Goldsmith

8:50 COLL 796. Balancing multiple orthogonal functions simultaneously on a single surface. **T. Lawton**, J.R. Uzarski, S. Filocamo

9:10 COLL 797. Optimization of micro/nanocapsules attachment by tailoring the surface nature of textiles. W. Akbar, R. Ihnfeldth, **G. Basim**

9:30 COLL 798. Determining optimum surface preparations to control the selectivity of ethanol chemistry over TiO_2/Au(111). **A. Baber**, D. Boyle, J. Wilke, V.H. Lam

9:50 COLL 799. Directing and morphing bouncing water droplets using chemically patterned surfaces. T. Dong, **T.J. McCarthy**

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

10:10 COLL 800. Rapid covalent surface modifications using the Piers-Rubinsztajn reaction. **D. Flagg**

10:30 COLL 801. Single-nanogap level characterization of ultra-dense Nanogap-Enhanced Raman Scattering (NERS) array surface. **Y. Suh**

10:50 COLL 802. Reactions of persistent carbenes with silicon surfaces. **A.V. Zhukhovitskiy**, M. Mavros, K.L. Queeney, T. Wu, T.A. Van Voorhis, J.A. Johnson

11:10 COLL 803. On the role of non-bulk interfacial structures in rutile-anatase TiO2 interfaces. **M. Nolan**, K.A. Gray

11:30 COLL 804. *In situ* chemical imaging of energy and environmental interfaces. **X. Yu**

11:50 COLL 805. $CuInS_2$-ZnS-based electro optic devices: Surface, surface and surface. **G. Zaiats**, J.B. Hoffman, S. Kinge, P.V. Kamat

Section D

Moscone Center

2008

Hierarchical Self-Assembly of Organic Monolayers, Bilayers & Films: Theory & Experiment

A. H. Flood, *Organizer*

S. L. Tait, *Organizer, Presiding*

8:30 COLL 806. From standing to sitting: Leveraging iterative phase segregation to create hierarchically nanostructured synthetic materials. **S.A. Claridge**

8:50 COLL 807. Effect of the first layer on polyelectrolyte multilayer structure. **X. Lyu**, A.M. Peterson

9:10 COLL 808. Partitioning of organic solutes into bilayers formed by non-ionic surfactants. **J. Siepmann**, M.S. Minkara, R.K. Lindsey, S.N. Jamadagni, D.M. Eike, P.H. Koenig

9:40 COLL 809. Beyond self-assembly: 2D chemical interactions and patterns, a computational approach to complex systems. **F. Zerbetto**

10:10 COLL 810. Understanding polymorphic accessibility and stability in molecular semiconductor thin films. **Y. Loo**

10:40 COLL 811. Principles and applications of grazing incidence small angle and wide angle x-ray scattering. **B. Lee**

11:10 COLL 812. Rational design of block copolymer compatablizers for ternary blend polymer bulk heterojunction solar cells. D. Kipp, R. Verduzco, **V. Ganesan**

11:40 COLL 813. Nano-phase behavior of surface-adsorbed, monodisperse oligodimethylsiloxane-based block molecules. **J. Teyssandier**, J.A. Berrocal, B. de Waal, E.W. Meijer, S. De Feyter

12:00 COLL 814. Fast, facile, and scalable fabrication of slippery liquid-infused surfaces using layer-by-layer assembly enabled by in-situ proton transfer. **G.H. Zhu**, N. Zacharia

Section E

Moscone Center

2010

Basic Research in Colloids, Surfactants & Nanomaterials

Self-Assembly

R. Nagarajan, *Organizer*

K. Sakurai, *Presiding*

8:30 COLL 815. Platonic micelles: Glutamic acids bearing calix[4]arene micelle: pH-controllable aggregation number corresponding to regular polyhedra. **S. Fujii**, K. Sakurai

8:50 COLL 816. Platonic micelles: Thermodynamic consideration of the micelles with the discrete aggregation numbers and mon-dispersity. **K. Sakurai**

9:10 COLL 817. Synthesis of epoxy-functional diblock copolymer nano-objects via polymerisation-induced self-assembly and their use as Pickering emulsifiers. **F. Hatton**, K. Thompson, S.P. Armes

9:30 COLL 818. Time-resolved small-angle x-ray scattering studies of the micellar nucleation event during polymerization-induced self-assembly. **M.J. Derry**, O. Mykhaylyk, S.P. Armes

9:50 COLL 819. pH-resolved self-assembly of microbial glycolipids: Mechanicistic insights. **N. Baccile**

10:10 COLL 820. Hydrogen bonding asymmetric star-shape derivative of bile acid leads to supramolecular fibrillar aggregates that wrap into micrometer spheres. **T.T. Myllymäki**

10:30 COLL 821. Self-assembly of zwitterionic sulfobetaine siloxane onto silica nanoparticles for application as a versatile antifouling coating system. **B. Knowles**, P. Wagner, S. Maclaughlin, M. Higgins, P. Molino

10:50 COLL 822. Self-assembled protein vesicles made from recombinant fusion proteins. **Y. Jang**, W. Choi, J. Champion

11:10 COLL 823. Novel readily biodegradable disulfonate surfactants. **W. Yu**, Y. Cheng, E. Daugs, A. Argenton

11:30 COLL 824. Novel liposome-based Surface Enhanced Raman spectroscopy (SERS) substrate. **W. Lum**, I. Bruzas, Z. Gorunmez, S. Unser, L. Sagle

11:50 COLL 825. Block copolymer templated mono- and bimetallic catalysts for fuel cell electrocatalysis. **D.A. Rider**

Section F

Moscone Center

2012

Basic Research in Colloids, Surfactants & Nanomaterials

Metal Nanomaterials

R. Nagarajan, *Organizer*

L. Cademartiri, *Presiding*

8:30 COLL 826. Initial growth of Au nanostructures on TiO_2(110)-1x1 surface at elevated temperature. **X. Tong**

8:50 COLL 827. Polymer-like nanowires. **L. Cademartiri**

9:10 COLL 828. Functional and structural characterization of multi-functional gold nanoparticles. **L. Calzolai**, R. Capomaccio, I. Ojea Jimenez, D. Gilliland

9:30 COLL 829. Frugal innovation: Synthesis and applications of undercooled metal particles. i. Tevis, J. Chen, C. Frankiewicz, A. Martin, **M. Thuo**

9:50 COLL 830. Withdrawn.

10:10 COLL 831. Chemical identity of surfactants control the electronic behaviors of the metallic core in gold nanoparticles. **B.J. Lear**, A. Cirri

10:30 COLL 832. Assessment of the physical stability of metal and metal oxide films for enhanced signal detection in colorimetric bioassays. **E. Bonyi**, Z. Kukoyi, O. Daodu, K. Aslan

10:50 COLL 833. Size and shape dissolution of silver nanoparticles. **Y. Hu**, Q. Zhang, V. Colvin

11:10 COLL 834. Hidden electrostatic asymmetry of gold nanorods. **J. Kim**, M. Lien, M. Han, S. Magonov, Y. Zhu, H. Ferguson, J. Schotland, Y. Chang, T. Norris, N. Kotov

11:30 COLL 835. Comparative roles of Zr(IV) and Ni(II) hetero-metal substituted polyoxometalates in oxidation solutions. **S.L. Giles**, J. Lundin, P.E. Pehrsson, R.B. Balow, W.O. Gordon, G.W. Peterson, B.T. Rasley, J.H. Wynne

11:50 COLL 836. Multi-stage transformation and lattice fluctuation at AgCl-Ag nanoparticle interface. **J.S. Du**, J. Park, Q. Kim, V.P. Dravid, D. Yang, D.A. Weitz

Section G

Moscone Center

2001

Basic Research in Colloids, Surfactants & Nanomaterials

Nanomaterials

R. Nagarajan, *Organizer*

K. C. Tvrdy, *Presiding*

8:30 COLL 837. Novel sol-gel derived TiO_2-SiO_2 particle systems for direct ink writing compositionally tailored GRIN glasses. **J.F. Destino**, T. Yee, N. Dudukovic, C. Meyers, D. Nguyen, E. Duoss, R. Dylla-Spears

8:50 COLL 838. New algorithm to model quantum growth dot dynamics. **K.C. Tvrdy**, N. Weeks

9:10 COLL 839. Damping of quantum dot acoustic phonons by chalcogenide surface ligands. **K. Schnitzenbaumer**, G. Dukovic

9:30 COLL 840. Microfluidic discovery platform: Toward nanoparticle functionalization through closed loop optimization. **K. Park**, S. Izor, J.D. Watt, D. Huber, D.H. Wang, L. Tan, R.A. Vaia

9:50 COLL 841. First steps in the Fischer-Tropsch reaction catalyzed by ultra-small ruthenium nanoparticles: A DFT study. L. Cusinato, L.M. Martínez-Prieto, B. Chaudret, I. Del Rosal, **R. Poteau**

10:10 COLL 842. Magnetic nanoparticles as contrast agents for reservoir imaging. **S. Al Hassan**, M. Subrati, G. Papavassiliou, D. Gournis, S. Pantelides, H. Kim

10:30 COLL 843. Characterization of nanoparticle interactions and thin film properties using MP-SPR. N. Granqvist, **A. Jokinen**, J. Kuncova-Kallio, J.W. Sadowski

10:50 COLL 844. Controlled nanoparticle morphology transitions induced by high-pressure ice-segregation. **J. Snitker**, M.O. Montes

11:10 COLL 845. Inorganic-organic hybrid electrical devices based on nanoparticle arrays for switchable current and spin transport. **R.C. Bruce**, C.A. Hacker

11:30 COLL 846. 2μm Ultrathin silica shells doped with iron (III) for low threshold of CPS and color doppler ultrasound performace and notable biodegradability. **C. Huang**, J. Yang, J. Wang, J. Oviedo, W.C. Trogler, A. Kummel, M. Kim

Section H

Moscone Center

2003

Basic Research in Colloids, Surfactants & Nanomaterials

Colloids in Environment & General Papers

R. Nagarajan, *Organizer*

K. Mandel, *Presiding*

8:30 COLL 847. Superparamagnetic carrier particles for water purification, resources recovery and substance sensing in fluids. **K. Mandel**

9:00 COLL 848. Colloidal gold nanorods uptake study on *C. fluminea* filter-feeding bivalve clams: Effect of aspect ratio and surface coating. **S. Abtahi**, P.J. Vikesland, C.J. Murphy, N.B. Saleh

9:20 COLL 849. Plasma modified catalytic micromotors. **L. Oksuz**, G. Yurdabak Karaca, E. Uygun, U. Koc, F. Kuralay, A. Uygun Oksuz

9:40 COLL 850. Thermochemistry of MAX and MXene phases. **G. Sharma**, M. Naguib, D. Feng, Y. Gogotsi, A. Navrotsky

10:00 COLL 851. Incorporating oxygenates into diesel fuel systems via stable reverse micelles. M. Webb, T. Riiff, W.J. Orts, **K. Aramthanapon**

10:20 COLL 852. Effect of viscosity on the propulsive motion of catalytic Janus motors. **P. Chatterjee**, E. Tang, P. Underhill

10:40 COLL 853. Manipulating single molecular junctions using electrochemical environments. **Y. Zang**, M.S. Inkpen, L. Venkataraman

11:00 COLL 854. Effect of moisture on the hydrolysis of basic salts. **X. Shi**, K. Lackner

11:20 COLL 855. Moisture-swing thermodynamics. **H. Azarabadi**, K. Lackner

Section I

Moscone Center

2005

Basic Research in Colloids, Surfactants & Nanomaterials

Synthesis of Colloids & in Colloidal Media

R. Nagarajan, *Organizer*

M. Stefik, *Presiding*

8:30 COLL 856. Organometallic route to layered zinc hydroxides and their exfoliated monolayers in apolar solvents. **A. Leung**, S.D. Pike, A.J. Clancy, H. Yau, M. Shaffer, C.K. Williams

8:50 COLL 857. Precision tunable nanomaterials from persistent micelle templates. **M. Stefik**

9:10 COLL 858. Facile, single-pot preparation of nanoporous silica with AgNPs at the core and curst for controlled Ag^+ ion release. **M. Salman Haider**, G.N. Shao, K. Hee Taik

9:30 COLL **859.** Selective electropolymerization of aniline on an ITO electrode using magnetic nanoparticles and a varying magnetic field. **D. Wirth**

9:50 COLL **860.** Morphology, structure, and optical properties of 2D SnS nanoplates synthesized via a hot-injection method. **N. Trejo**, A. Hunter, M. Nguyen, C. Wrasman, J. Dwyer, E.S. Aydil

10:10 COLL **861.** Synthesizing and screening high mobility nanoparticles. **D. Garcia-Rojas**, G. Escalera, A. Mendoza-Garcia, C. Masterson, V. Colvin

10:30 COLL **862.** Surfactant-induced shape changes in oil droplets caged in deformable polymer shells as templates for the synthesis of anisotropic polymer particles. **X. Guo**, N.L. Abbott, D.M. Lynn

10:50 COLL **863.** Synthesis and chemical transformation of nickel nanoparticles embedded in silica. **B.B. Lynch**, B.D. Anderson, W.J. Kennedy, J.B. Tracy

11:10 COLL **864.** Carboxylate decomposition: A critical step in high temperature synthesis of metal oxide nanocrystals. **C. Masterson**, A. Mendoza-Garcia, V. Colvin

11:30 COLL **865.** Synthesis and characterization of metal-doped synthetic melanin nanoparticles. **Z. Wang**, Y. Li, Y. Huang, N.C. Gianneschi

11:50 COLL **866.** Effect of solution composition on Pu oxide nanoparticle morphology. **T. Parsons-Moss**, J. Shusterman, D. Olive, Z. Dai, M. Zavarin, A. Kersting

Bio-based Gels & Porous Materials

Aero-, Cryo- & Xerogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms: Metals

Sponsored by CATL, Cosponsored by COLL and ENVR

Oxides

Sponsored by CATL, Cosponsored by COLL and ENVR

Functional Lignocellulosics & Nanotechnology

Responsive Materials & Biosensors

Sponsored by CELL, Cosponsored by CARB and COLL

THURSDAY AFTERNOON

Bio-based Gels & Porous Materials

Open-Porous Carbon Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Elucidation of Mechanisms & Kinetics on Surfaces

Oxidation Reactions

Sponsored by CATL, Cosponsored by COLL and ENVR

Beyond Hydrocarbons

Sponsored by CATL, Cosponsored by COLL and ENVR

Functional Lignocellulosics & Nanotechnology

(nano)Paper: From Fundamentals to Applications/Antimicrobial, Functional Materials

Sponsored by CELL, Cosponsored by CARB and COLL

COMP

Division of Computers in Chemistry

H. Woodcock, M. Feig and J. Shen, *Program Chairs*

BUSINESS MEETINGS:

Business Meeting, 3:00 PM: Sat

SOCIAL EVENTS:

Social Hour, 7:00 PM: Sat

SUNDAY MORNING

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Allosteric Regulation & Mechanisms

Cosponsored by PHYS

C. Chang, *Organizer*

G. Verkhivker, *Organizer, Presiding*

8:30 Introductory Remarks.

8:45 COMP **1.** Allosteric mechanisms in receptor function and modulation: Toward a new pharmacology. **J. Changeux**

9:30 COMP **2.** Allosteric functional mechanisms of molecular machines in the cell membrane. **H. Weinstein**, M.V. LeVine, G. Khelashvili, M.A. Cuendet, A. Razavi

10:00 COMP **3.** Allostery driven by metal ions: Getting transition metal ions around cells safely. **K.M. Merz**

10:30 Intermission.

10:50 COMP **4.** Dissecting and controlling protein allostery. **N. Dokholyan**

11:20 COMP **5.** Entangled relationships: Protein flexibility, allostery, and mutation. **D. Livesay**

11:50 COMP **6.** Toward rational allosteric engineering of molecular motor and switch protein function. **B. Grant**

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

K. Honkala, B. Liu, *Organizers*

B. Liu, *Presiding*

8:30 COMP **7.** Advances in density functional theory for molecules and materials. N. Mardirossian, **M.P. Head-Gordon**

9:05 COMP **8.** New discovery tools for transition metal catalyst design. T.Z. Gani, J.P. Janet, E. Ioannidis, **H.J. Kulik**

9:40 COMP **9.** Automated surface structure determination and reaction path identification. **B. Hammer**

10:15 Intermission.

10:35 COMP **10.** Formation and structure of black anatase TiO_2: A combined force field and first principles study. S. Selcuk, X. Zhao, **A. Selloni**

11:10 COMP **11.** Discovery of new polymer photocatalysts for water splitting: The role of computational chemistry. P. Guiglion, A. Monti, **M.A. Zwijnenburg**

11:45 COMP **12.** Theoretical water splitting mechanisms on manganese oxide clusters. **C.M. Aikens**, A. Fernando, M. Just, K. Skinner, A.Z. Clayborne, T.N. Haddock

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

G. Gidofalvi, E. Hohenstein, *Organizers*

A. E. DePrince, *Organizer, Presiding*

8:30 COMP **13.** On-the-fly CASPT2 nonadiabatic dynamics. **T. Shiozaki**

9:10 COMP **14.** Reaching towards FeMoCo. Z. Li, S. Guo, A. Sokolov, **G.K. Chan**

9:50 COMP **15.** Reduced-order formulation of multi-reference perturbation theory via tensor hyper-contraction. **C. Song**, T.J. Martinez

10:15 Intermission.

10:30 COMP **16.** Coupled cluster theory for hundreds of atoms. **F. Neese**

11:10 COMP **17.** Generalized active space method for affordable multi-reference calculations. **L. Gagliardi**

11:50 COMP **18.** Construction of R12 geminal-projected particle-hole creation operators for many-electron systems using diagrammatic factorization approach. M.G. Bayne, **A. Chakraborty**

Section D

InterContinental San Francisco

Cathedral Hill

Computational Studies of Water

D. J. Sindhikara, *Organizer*

V. Mouchlis, *Presiding*

8:30 COMP **19.** Thermodynamic characterization of water in biomolecular recognition. R. Abel, S. Mondal, C. Masse, J. Greenwood, G. Harriman, M. Ashwell, S. Bhat, **T. Beuming**, R. Wester, L. Frye, R. Kapeller, R. Friesner

9:10 COMP **20.** Protein hydration free energies in explicit vs implicit solvent - a direct comparison. **P. Setny**

9:40 COMP **21.** Testing a desolvation term in molecular docking on a model cavity. **T.E. Balius**, M. Fischer, R.M. Stein, T.B. Adler, C.N. Nguyen, A. Cruz, M.K. Gilson, T.P. Kurtzman, B. Shoichet

10:10 Intermission.

10:25 COMP **22.** Conserved H_2O in protein-ligand complexes: An evaluation of water prediction tools. **E. Nittinger**, P.A. Gibbons, V. Tsui, M. Rarey, D.F. Ortwine

10:50 COMP **23.** Water prediction validated by x-ray crystallography in the B1 domain of neuropilin-1. **A. Chan**

11:15 COMP **24.** Comparing water dynamics in cryo-EM and x-ray derived molecular models. **F. Tofoleanu**, F.C. Pickard, S. Subramaniam, B. Brooks

11:40 COMP **25.** Toward a force-field validation engine: Attach-Pull-Release calculations of host-guest binding thermodynamics. **J. Yin**, M.K. Gilson

Section E

InterContinental San Francisco

Laurel Hill

Computer-Aided Peptide Design

In-Silico Peptide Modeling

Cosponsored by CINF

Q. Deng, S. N. Ha, *Organizers*, *Presiding*

8:30 COMP **26.** BRIKARD: A kinematics-based algorithm for the conformational sampling and design of macrocycles. **E. Coutsias**

9:00 COMP **27.** Computational modeling of cyclic peptides. S. McHugh, D. Slough, H. Yu, J. Rogers, **Y. Lin**

9:30 COMP **28.** Fragment-centric topographical mapping of protein-peptide interaction interfaces. **Y. Zhang**

10:00 Intermission.

10:15 COMP **29.** Relative binding free energies from flexible peptide binding simulations. **A. Perez**, J.A. Morrone, Q. Deng, S.N. Ha, K. Dill

10:45 COMP **30.** Recent advances in structure-based prediction of protein-peptide binding affinities. **T. Beuming**, H. Li, E. Feyfant

11:15 COMP **31.** Stapled peptides: Specific reagents, potential therapeutics. **C. Verma**

Section F

InterContinental San Francisco

Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, J. M. Blaney, *Organizers*

E. Metwally, V. Shanmugasundaram, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 COMP **32.** Computational & data sciences in the cloud – To be or not to be. **R.K. Kondru**

9:05 COMP **33.** Lessons learned in using Cloud BigCompute to transform computational chemistry research. **J. Stowe**

9:35 COMP **34.** Getting our heads into the cloud: GSK experiences using cloud computing for structure based drug design. **A.P. Graves**

10:05 Intermission.

10:20 COMP **35.** Practical lessons learned on a long and winding road to The Cloud. **N.P. Labello**, G.A. Bakken

10:50 COMP **36.** Design anywhere: A mobile app for drug design. **H. Zhang**, J. Lajiness, J. Hughes, M. Lajiness, J. Wang

‡ *Cooperative Cosponsorship*

11:20 COMP **37.** Accelerating discovery in the cloud: A cohesive workflow for the virtual screening and refinement of computationally-intensive libraries. **E. Metwally**

Materials Informatics & Computational Modeling

Sponsored by CINF, Cosponsored by COMP and POLY

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Simulating Electrons on Large Scale

Sponsored by PHYS, Cosponsored by COMP

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

SUNDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Undergraduate Research & National Meeting Roundtable

E. C. Sherer, *Organizer*

M. C. Nagan, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 COMP **38.** Introduction to quantum chemistry. **A.E. DePrince**

2:25 COMP **39.** Molecular mechanics in computational chemistry: An overview for undergraduates. **C.L. Simmerling**

3:15 Discussion.

4:05 Intermission.

4:20 Panel Discussion.

5:10 Concluding Remarks.

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

B. Liu, *Organizer*

K. Honkala, *Organizer, Presiding*

1:30 COMP **40.** Insight into catalyst activity and selectivity drawn from molecular modeling. **A.T. Bell**

2:05 COMP **41.** First-principles based multiscale multiparadigm methods with applications to complex material. **W.A. Goddard**

2:40 COMP **42.** First principles kinetic modeling of methane oxidation over Pd and PdO. M. Jorgensen, M. Van den Bossche, **H. Gronbeck**

3:15 Intermission.

3:35 COMP **43.** Mechanism of CO and CO_2 hydrogenation over copper-based catalysts. **F. Studt**

4:10 COMP **44.** Crystal phase effect on CO activation for Fischer-Tropsch synthesis. J. Liu, **W. Li**

4:45 COMP **45.** Gold particle size effect for CO oxidation: A first-principles study. **J. Liu**, E. Hensen, I. Filot

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, G. Gidofalvi, *Organizers*

E. Hohenstein, *Organizer, Presiding*

1:30 COMP **46.** Accurate nonadiabatic dynamics. **D.R. Yarkony**

2:10 COMP **47.** Painless modeling of dynamics near conical intersections. **B.G. Levine**, G.A. Meek

2:50 COMP **48.** Energy dissipation at metal surfaces: The surprisingly high non-adiabaticity of Na diffusion on Cu(111). **S.P. Rittmeyer**, K.U. Reuter

3:15 Intermission.

3:30 COMP **49.** Dynamics of electron transfer near a metals surface. **J.E. Subotnik**, W. Dou, W. Ouyang

4:10 COMP **50.** Single-reference dynamics of strongly correlated systems: How far can we go? **M. Barbatti**

4:50 COMP **51.** New theoretical approaches to simulate photoinduced proton-coupled electron transfer reactions. **P. Huo**

Section D

InterContinental San Francisco

Cathedral Hill

Computational Studies of Water Binding & Biology

D. J. Sindhikara, *Organizer*

F. L. Kearns, *Presiding*

1:30 COMP **52.** Methods and models for condensed phase simulation of water. **T.L. Head-Gordon**

2:00 COMP **53.** Capturing dynamics, along with thermodynamics, in the Implicit Solvent using the SuperPosition Approximation (IS-SPA) model. **P.T. Lake**, M. McCullagh

2:30 COMP **54.** Good from far, far from good: Comparing quantum and classical hydration of model ions. **R.C. Remsing**

3:00 Intermission.

3:15 COMP **55.** Modeling radical interactions with water. **J. Arey**, P. Tentscher

3:35 COMP **56.** New dissociative water model. **O. Akin-Ojo**

3:55 COMP **57.** Rate theory in two-dimensional reaction coordinate space: Applications to ion-pairing. **S. Roy**, M.D. Baer, C.J. Mundy, G.K. Schenter

4:15 COMP **58.** Enhanced modeling of water in two-dimensions with rose potentials. **C.J. Fennell**

4:35 COMP **59.** How to model chemical reactions in electrolytes? **S. Ringe**, H. Oberhofer, K.U. Reuter

Section E

InterContinental San Francisco

Laurel Hill

Computer-Aided Peptide Design

Computational Approaches to Peptide ADME

Cosponsored by CINF

Q. Deng, S. N. Ha, *Organizers*, *Presiding*

1:30 COMP **60.** ADME analysis of therapeutic peptides: Preserving product value. **J.H. Hochman**

2:00 COMP **61.** Factors for governing cell permeability and oral bioavailability in macrocycles. **S. Lokey**

2:30 COMP **62.** High throughput method for the indirect detection of intramolecular hydrogen bonding. **S. Sciabola**

3:00 Intermission.

3:15 COMP **63.** Property trends among permeable cyclic peptides. **A. Mathiowetz**

3:45 COMP **64.** Mechanism-based ADME/PK prediction, with applications to macrocycles. **M.P. Jacobson**

4:15 COMP **65.** Design of technology-compatible cyclic peptide scaffolds with oral bioavailability. **A. Golosov**

4:45 COMP **66.** PepSee — A new tool for peptide analysis & design. **M. Gastreich**, M. Skovgaard

Section F

InterContinental San Francisco

Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, E. Metwally, *Organizers*

J. M. Blaney, V. Shanmugasundaram, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 COMP **67.** Cloud first strategy that accelerates informatics and computations in drug discovery. **J. Feng**

2:05 COMP **68.** High performance and/or cloud computing for free energy prediction using molecular dynamics simulations? S. Wan, D.W. Wright, S.J. Zasada, A.P. Bhati, **P.V. Coveney**

2:35 COMP **69.** Lessons learned in developing and delivering a secure, multi-tenant environment for drug discovery R&D informatics. **W.W. Smith**, B.A. Bunin

3:05 Intermission.

3:20 COMP **70.** What's with all this GPU-accelerated cloud computing stuff? **M.E. Berger**

3:50 COMP **71.** Cloud is the only place for computational chemistry: Why this is a once-in-a-lifetime opportunity for the field to leap forward. **P.C. Hawkins**, A.G. Skillman, R. Tolbert, J. LaFon, C. Bruce, A. Nicholls

4:20 COMP **72.** Enhancing internal computational capabilities with the cloud. **J. Duca**, D. Chin, C. Hajdin, S. Litster

Materials Informatics & Computational Modeling

Sponsored by CINF, Cosponsored by COMP and POLY

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Simulating Quantum Nuclei on Large Scale

Sponsored by PHYS, Cosponsored by COMP

Computations for CO_2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY MORNING

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

Z. Luthey-Schulten, *Presiding*

8:30 COMP **73.** Energy landscape theory: From folding to function in genetic networking. **P.G. Wolynes**

9:00 COMP **74.** Touring the protein folding landscape: The view depends on how and where you look. **S. Marqusee**

9:30 COMP **75.** Exploring allostery from protein folding to function using coarse-grained models. **C.L. Brooks**

10:00 Intermission.

10:20 COMP **76.** Exploring protein function: The convergence of structure based models and co-evolutionary information. **J.N. Onuchic**

10:50 COMP **77.** Significance of neuronal structural complexity and spatial heterogeneity in modulating dopamine reuptake dynamics. C. Kaya, M.H. Cheng, E. Block, T. Bartol, T. Sejnowski, A. Sorkin, J.R. Faeder, **I. Bahar**

11:20 COMP **78.** Exploring fitness and free energy landscapes of proteins for allostery and binding. **R.M. Levy**

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

K. Honkala, *Organizer*

B. Liu, *Organizer, Presiding*

8:30 COMP **79.** First-principles modeling and design of catalytic materials. **P. Sautet**

9:05 COMP **80.** Electroreduction of CO_2 to hydrocarbons and alcohols. **E. Skulason**, J. Hussain, H. Jonsson

9:40 COMP **81.** Engineering metal/SnOx interfaces for electrochemical CO_2 reduction. **H. Xin**, S. Wang

10:15 Intermission.

10:35 COMP **82.** Structure, stability, and reactivity of nano-structured oxides supported on metals. **A. Vojvodic**

11:10 COMP **83.** Toward modeling practical catalysis from first principles. W. An, Y. Liang, H. Kim, S. Liu, **P. Liu**

11:45 COMP **84.** Electrochemical reduction of nitric oxide on Pt-surfaces: A combined DFT and kMC approach. H. Chun, V. Apaja, **A.Z. Clayborne**, J.P. Greeley, K. Honkala

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, E. Hohenstein, *Organizers*

G. Gidofalvi, *Organizer, Presiding*

8:30 COMP **85.** DMRG: Orbital selection, dynamic correlation, and nuclear gradients. **M. Reiher**

9:10 COMP **86.** Wavefunction forms based on identities from combinatorics. **P. Ayers**

9:50 COMP **87.** Coupled-Cluster Valence Bond Singles and Doubles (CCVB-SD): Block-tensor based implementation and application to polyacenes. **J. Lee**, D. Small, M.P. Head-Gordon

10:15 Intermission.

10:30 COMP **88.** New vistas on the strong correlation problem. **G.E. Scuseria**

11:10 COMP **89.** Perturbative multireference similarity renormalization group approaches for ground and excited states. C. Li, K.P. Hannon, **F.A. Evangelista**

11:50 COMP **90.** GPU-accelerated state-averaged complete active space self-consistent field and derivative methods enable accurate, large-scale nonadiabatic dynamics simulations. **J.W. Snyder**, E. Hohenstein, B. Curchod, B. Fales, R.M. Parrish, T.J. Martinez

Section D

InterContinental San Francisco

Cathedral Hill

Computational Studies of Water Phenomena & Properties

D. J. Sindhikara, *Organizer*

T. E. Balius, *Presiding*

8:30 COMP **91.** Water structuring above planar hydrophobic surfaces. **U. Schnupf**, J. Brady

8:55 COMP **92.** Monte Carlo simulations probing the liquid/vapor interface of water/hexane mixtures. **M.S. Minkara**, D.J. Stein, C.J. Peters, J. Siepmann

9:20 COMP **93.** Surface potential of water with *ab initio* molecular dynamics. **T.T. Duignan**, M.D. Baer, G.K. Schenter, C. Mundy

9:45 COMP **94.** Deviation of the surface tension of water suggests the possible emergence of a new form of liquid upon supercooling. **F. Wang**

10:10 Intermission.

10:25 COMP **95.** Modelling the refractive index of the air-water interface. **F. Longford**, J.W. Essex, C. Skylaris, J.G. Frey

10:45 COMP **96.** Understanding the sensitivity of nucleation free energies to the molecular model in water and ion/water systems. **S.J. Keasler**, M.A. Olson, J. Schlecht, S. Pavlenko, J. Siepmann

11:05 COMP **97.** Hydrophobic polymer collapse: Unravelling molecular mechanisms for osmolyte protection and denaturation. **N. van der Vegt**

11:25 COMP **98.** Fluctuation phenomena and structure of revPBE water at ambient and high pressure (up to 360 MPa). **M. Galib**, G.K. Schenter, J. Fulton, C.J. Mundy

11:45 COMP **99.** Predictive description of electronic properties in aqueous solutions. **T. Pham**, M. Govoni, R. Seidel, S.E. Bradforth, E. Schwegler, G.A. Galli

Section E

InterContinental San Francisco

Laurel Hill

Drug Design

Docking & Protein-Ligand Interaction Analysis

M. R. Landon, Y. Tseng, *Organizers*

T. Abramyan, *Presiding*

8:30 COMP **100.** Protein-ligand scoring with convolutional neural networks. **D. Koes**, M. Ragoza, E. Idrobo, J. Hochuli, J. Sunseri

8:55 COMP **101.** Predicting hot and warm spots on proteins for fragment binding. **P. Rathi**, F. Ludlow, R.J. Hall, C. Murray, P. Mortenson, M. Verdonk

9:20 COMP **102.** PlayMolecule DeepSite: Protein binding site detector using 3D convolutional neural networks. **G. De Fabritiis**

9:45 Intermission.

10:05 COMP **103.** Understanding protein-ligand binding at the molecular level: Using swap-based methods to visualise binding free energy components. **C.J. Woods**, M. Malaisree

10:30 COMP **104.** Docking - old hat or hats off. **C. Lemmen**, C. Detering, M. Gastreich

10:55 COMP **105.** Interrogating protein ligand interactions– Knowledge base from PDB/CSD and energy decomposition methods. **J.H. Voigt**, U. Schmitz

11:20 COMP **106.** Development of a novel CHARMM-based flexible receptor-flexible ligand docking procedure. S.K. Vankayala, J.D. Larkin, **H.L. Woodcock**

Section F

InterContinental San Francisco

Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, V. Shanmugasundaram, *Organizers*

J. M. Blaney, E. Metwally, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 COMP **107.** Steps to getting science in the cloud at Merck. **R. Pete**, S.A. Johnson, B. Sherborne

9:05 COMP **108.** Deploying large-scale binding-affinity calculations to the cloud. **B.T. Hannigan**

9:35 COMP **109.** Xcellerate informatics: A cloud-based solution for clinical data integration and real-time monitoring of clinical trials. **D.K. Agrafiotis**

10:05 Intermission.

10:20 COMP **110.** Cyrus's journey to the cloud: How we got there and what we've learned. **L. Nivon**

10:50 COMP **111.** Distributed computing resources, from grid to cloud: Welcome to the HPC world! **E. Arnoult**

11:20 COMP **112.** Druggability assessment of the structural proteome with inclusion of light protein flexibility. **A.C. Cheng**, F. Boulnois, K. Loving, A. Lin

Advances in High-Throughput Screening

Sponsored by CINF, Cosponsored by COMP and MEDI

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Ab Initio & DFT

Sponsored by PHYS, Cosponsored by COMP

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

I. Bahar, *Presiding*

1:30 COMP **113.** Allosteric effects of weak transient protein-protein interactions: Crowding in cells and evolutionary consequences. **E. Shakhnovich**, S. Bhattacharyya, S. Bershtein

2:00 COMP **114.** Ribosome biogenesis in replicating cells: Integration of experiment and theory. **Z. Luthey-Schulten**

2:30 COMP **115.** Systematic perturbation of a fundamental biological switch. **T. Kortemme**

3:00 Intermission.

3:20 COMP **116.** Role of electrostatics in allosteric regulation. **M.P. Jacobson**

3:50 COMP **117.** Molecular principles for optimizing protein-DNA interactions. **K. Levy**

4:20 COMP **118.** Mediation of allosteric communication by inter-domain bridges. J. Guo, C. Guo, **H. Zhou**

4:50 COMP **119.** Phospholipase A2: A unique paradigm of allosteric regulation by membranes. **V. Mouchlis**, J. McCammon, E.A. Dennis

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

K. Honkala, B. Liu, *Organizers*

A. Z. Clayborne, *Presiding*

1:30 COMP **120.** Catalyst design on the computer. **J.K. Norskov**

2:05 COMP **121.** Static or dynamic? A first-principles multiscale modeling perspective on the nature of the surface of operating catalysts. **K.U. Reuter**

2:40 COMP **122.** First principles analysis of reactivity trends at the interface between metal nanoparticles and doped oxide supports. **J. Greeley**, T.S. Choksi, P. Majumdar, Z. Zhao, Y. Cui, W.F. Schneider, F. Ribeiro

3:15 Intermission.

3:35 COMP **123.** Catalysis of ice formation. **A. Michaelides**

4:10 COMP **124.** First-principles insights to the CO oxidation on oxidized Rh. **A. Hellman**

4:30 COMP **125.** Group additivity for adsorbed polyols at a Pt(111) surface under aqueous conditions. **B. Schweitzer**, G. Gu, S. Steinmann, C. Michel, P. Sautet, D.G. Vlachos

4:50 COMP **126.** General structure-activity relationships for transition metal oxides. **V. Fung**, F. Tao, D. Jiang

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, G. Gidofalvi, *Organizers*

E. Hohenstein, *Organizer, Presiding*

1:30 COMP **127.** Nonadiabatic dynamics of photoinduced proton-coupled electron transfer processes. **S. Hammes-Schiffer**

2:10 COMP **128.** Nonadiabatic molecular dynamics for spin-forbidden processes. D. Fedorov, R. Zaari, **S.A. Varganov**

2:50 COMP **129.** Can quantized vibrational effects be obtained from Ehrenfest mixed quantum-classical dynamics? **J.J. Goings**, D.B. Lingerfelt, X. Li

3:15 Intermission.

3:30 COMP **130.** Charge transfer dynamics, excited state energetics, and organic photovoltaics. **N. Ananth**

4:10 COMP **131.** Optomechanical control of photochemical quantum yields in a biological chromophore model. **M. Olivucci**, L. Frutos, A. Valentini

‡ *Cooperative Cosponsorship*

4:50 COMP **132.** Quantum dynamics in CS^+ collision with H using time dependent wave packet dynamics. **R. Kaur**, D. Thogluva

Section D

InterContinental San Francisco
Cathedral Hill

Data Science Challenges in Computational Chemistry

Cosponsored by CINF

M. Feig, *Organizer*

C. L. Simmerling, G. Vacek, *Organizers*, *Presiding*

1:30 COMP **133.** Meaningful state space discretization at the macro-cluster level. H. Liu, M. Li, J. Fan, **S. Huo**

2:00 COMP **134.** Building Markov state models of diffusion processes in many-particle systems from generic order parameters. **J.F. Rudzinski**, M. Radu, K. Kremer, T. Bereau

2:30 COMP **135.** Understanding and applying multistate reweighting in a broad molecular simulation context. **M.R. Shirts**

3:00 Intermission.

3:15 COMP **136.** Cluster analysis of molecular simulation trajectories for systems where both conformation and orientation of the sampled states are important. **T. Abramyan**, J. Snyder, A.A. Thyparambil, S. Stuart, R.A. Latour

3:45 COMP **137.** HTMD: High-throughput molecular dynamics for molecular discovery. **G. De Fabritiis**

4:15 COMP **138.** Geometric searching in large collections of protein-ligand interfaces. T. Inhester, E. Nittinger, **M. Rarey**

4:45 COMP **139.** Proper data extraction and curation in an era of linked open data – Are we there yet? **B. Zdrazil**, G.F. Ecker

Section E

InterContinental San Francisco
Laurel Hill

Drug Design

Computational Methods & Approaches

M. R. Landon, Y. Tseng, *Organizers*

J. L. Paulsen, *Presiding*

1:30 COMP **140.** Common hits approach: Combining pharmacophore modeling and molecular dynamics simulations. **M. Wieder**, A. Garon, U. Perricone, T. Seidel, S. Boresch, T. Langer

1:55 COMP **141.** Protein binding sites dynamics in drug discovery. **D. Janezic**, J. Konc

2:20 COMP **142.** New approaches for binding site and ligand prediction and their use in drug discovery. **J. Konc**, D. Janezic

2:45 Intermission.

3:05 COMP **143.** pmemdGT: An efficient and accurate GPU-accelerated thermodynamics integration simulation package. **T. Lee**, D.M. York

3:30 COMP **144.** Efficient free energy perturbation Hamiltonian replica exchange molecular dynamics method for absolute binding affinity predictions. **W. Jiang**

3:55 COMP **145.** Calculating the absolute binding free energies for octa-acids and guests. **F. Tofoleanu**, J. Lee, F.C. Pickard, G. Koenig, J. Huang, M. Baek, C. Seok, B. Brooks

4:20 COMP **146.** Hybrid quantum and classical free energies: Separating the wheat from the chaff with configuration space overlaps. **C. Cave-Ayland**, C. Skylaris, J.W. Essex

Section F

InterContinental San Francisco
Nob Hill

Should I Move My Computational Chemistry or Informatics Tools to the Cloud?

Cosponsored by CINF

R. Alvarez, E. Metwally, *Organizers*

J. M. Blaney, V. Shanmugasundaram, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 COMP **147.** Using the cloud for massive scale-up of computationally intensive physics-based simulations. **V. Eyrich**, J. Watney, Y. Zhao, L. Wang, S. Mondal, S. Bhat, R. Abel

2:05 COMP **148.** CHARMM interface and graphics: A flexible web-user interface for education and application of molecular simulation and multiscale modeling. J. Smock, V. Schalk, Y. Pevzner, B.T. Miller, **H.L. Woodcock**

2:35 COMP **149.** AceCloud: Molecular dynamics simulations in the cloud. M. Harvey, **G. De Fabritiis**

3:05 Intermission.

3:20 COMP **150.** Virtual screening in the cloud with Pharmit. **D. Koes**

3:50 COMP **151.** Research informatics: Get ready for the cloud! **M. Van Daelen**

4:20 Discussion.

4:40 Concluding Remarks.

Advances in High-Throughput Screening

Sponsored by CINF, Cosponsored by COMP and MEDI

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Semiempirical & DFTB

Sponsored by PHYS, Cosponsored by COMP

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

H. L. Woodcock, *Organizer*

8:00 - 10:00

236, 240-247, 261, 267, 277, 283-284, 286, 290, 305-306, 310-312, 331, 341, 345, 347, 349, 353-357, 360, 362, 365, 368, 375, 377, 383, 389-391, 396-398, 402-403, 406, 410, 416-417, 419, 421, 424, 426. See subsequent listings.

TUESDAY MORNING

Section A

InterContinental San Francisco
Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

H. Weinstein, *Presiding*

8:30 COMP **152.** Structural mechanisms of the allosteric regulation of Ras. **J. Kuriyan**

9:00 COMP **153.** Ancient origins of allosteric activation–Exploitation for novel cancer drugs. **D. Kern**

9:30 COMP **154.** Fractal nature of protein interior and its implications for allostery. **A. Kornev**, S.S. Taylor

10:00 Intermission.

10:20 COMP **155.** How EGF and insulin activate their receptors. **D. Leahy**, J. Kavran, P. Byrne

10:50 COMP **156.** Genetically tunable frustration controls allostery in an intrinsically disordered transcription factor. **V.J. Hilser**

11:20 COMP **157.** Role of intrinsically disordered proteins in allosteric regulation of cellular signaling. **P.E. Wright**

Section B

InterContinental San Francisco
Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

B. Liu, *Organizer*

K. Honkala, *Organizer, Presiding*

1:30 COMP **158.** Computational catalysis: Rigor and relevance. **J. Sauer**

2:05 COMP **159.** Diesel oxidation catalysts with improved low temperature activity identified from computational screening. Y. Song, J.S. Arevalo, W. Epling, **L. Grabow**

2:40 COMP **160.** Operando catalysis: Computing the state of a zeolite catalyst at reaction conditions. **W.F. Schneider**, C. Paolucci, H. Li, S. Li

3:15 Intermission.

3:35 COMP **161.** Complete catalytic cycle for fast and standard NH_3-SCR reaction. **H. Falsig**

4:10 COMP **162.** Understanding diffusion during catalytic fast pyrolysis of biomass over H-ZSM-5 by multiscale modeling. L. Bu, B. Knott, P.N. Ciesielski, M.R. Nimlos, D. Robichaud, **S. Kim**

4:30 COMP **163.** Adsorption and activation of water on cuboctahedral rhodium and platinum nanoparticles. **A.S. Bazhenov**, L. Lefferts, K. Honkala

4:50 COMP **164.** Structural study of the Ziegler-Natta catalyst. **V. D'Anna**, P. Sautet

Section C

InterContinental San Francisco
Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

A. E. DePrince, E. Hohenstein, *Organizers*

G. Gidofalvi, *Organizer, Presiding*

8:30 COMP **165.** Direct patching exchange-correlation potential in density functional theory. **C. Huang**

9:10 COMP **166.** Unpaired densities in singlet polyradicals: Local electron correlation treatment in extended multi-reference approaches in comparison with quasi correlated tight binding. **H. Lischka**

9:50 COMP **167.** Derivative coupling vectors from a Davidson approach. **J.A. Kammeraad**, P.M. Zimmerman

10:15 Intermission.

10:30 COMP **168.** Time-dependent two-component relativistic spin dynamics. **X. Li**

11:10 COMP **169.** Excited-state dynamics of mPlum flourecent protein. **S. Faraji**, A. Krylov

11:50 COMP **170.** Nonadiabatic couplings and the choice of density functional: Exchange cannot be neglected. **A.V. Akimov**

Section D

InterContinental San Francisco
Cathedral Hill

Molecular Mechanics

Sampling Long Time Scales

M. Feig, *Organizer*

J. V. Vermaas, *Presiding*

8:30 COMP **171.** Enhancing conformational sampling by modifying the underlying velocity distribution: Digitally filtered hybrid Monte Carlo. **C.S. Pervane**, J.W. Essex

8:55 COMP **172.** Novel enhanced sampling approach for cryptic site discovery on protein targets. **F. Gervasio**

9:25 COMP **173.** Rapid protocol for free energy calculations via multi-dimensional expanded ensemble simulations. **B. Radak**, B. Roux

9:55 Intermission.

10:10 COMP **174.** MS-Fold: Protein structure prediction guided by covalent labeling mass spectrometry data. M. Marlett, S.H. Hinckley, V.H. Wysocki, **S. Lindert**

10:40 COMP **175.** Fast free energy calculations from proximal distribution functions. **S. Ou**, B.M. Pettitt

11:10 COMP **176.** Unraveling the mechanistic basis of the CRISPR-Cas9 system via molecular simulations. **G. Palermo**, Y. Miao, R. Walker, M. Jinek, J. McCammon

11:40 COMP **177.** pH-dependent conformational change and its impact on *E.coli* glycinamide ribonucleotide transformylase catalytic activity. **P. Gupta**, A.E. Roitberg

Section E

InterContinental San Francisco

Laurel Hill

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Cosponsored by BIOL, MEDI and WCC

D. J. Kempf, Y. C. Martin, *Organizers*

T. R. Stouch, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 COMP **178.** QSAR: How my success relied on pillars built by Yvonne Connolly Martin. **G. McGaughey**

9:05 COMP **179.** Big data, small data: Pharmacology-based similarity measures and statistically-derived amino acid weightings to inform kinome selectivity. **M. Torrent**

9:30 COMP **180.** Integrated hit generation: Iterative design of experiments, screening sets, and compounds. **J.M. Jansen**, P.S. Lee, V.R. Polyakov, L. Tian, E.J. Martin

9:55 Intermission.

10:10 COMP **181.** Recent advances in applying computation to (bio) catalyst design. **K.W. Lexa**

10:35 COMP **182.** Innovation/evolution of cheminformatics evergreens. **M. Lee**

11:00 COMP **183.** Impact of quantitative drug design: Mighty oaks from little acorns grow. **M. Holloway**

11:25 Concluding Remarks.

Section F

InterContinental San Francisco

Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG‡

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

8:30 COMP **184.** Multi-scale modeling of nanomaterials: From DFT to molecular dynamics simulations. **F. Martin-Martinez**, Z. Qin, G. Jung, M.J. Buehler

8:55 COMP **185.** Reliable computational design of biological-inorganic materials to the large nanometer scale using INTERFACE-FF. **H. Heinz**

9:20 COMP **186.** Advances in atomic-scale methods for materials chemistry. **S.B. Sinnott**

9:45 COMP **187.** Inference-boosted first-principles molecular dynamics for chemo-mechanical modelling. **A. De Vita**

10:10 Intermission.

10:30 COMP **188.** Modeling the formation of sodium and calcium aluminosilicate gels at the mesoscale using coarse-grained Monte Carlo. **K. Yang**, C. White

10:45 COMP **189.** Simulations of polymer membranes with chain altering and conservative Monte Carlo moves. **A. Bick**, L. Subramanian

11:10 COMP **190.** Solvation and encapsulation of photoactive species: Insights from excited state DFTB. N. Garcia, A. Banducci, Z. Pollard, K. Komoto, **T. Kowalczyk**

11:35 COMP **191.** Recent DFTB extension for improving accuracy and boosting the efficiency for computational applications to nanomaterials. **T. Frauenheim**

12:00 COMP **192.** Entropy sampling for zeolite-catalyzed reactions at operating conditions. **K. De Wispelaere**, T. Bligaard, J.K. Norskov, V. Van Speybroeck

12:15 COMP **193.** Self-adaptive Reactive Force Fields (SERFF): Force matching for molecular dynamics simulation of reactive materials. **N. Goldman**

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Single Crystal Catalysis

Sponsored by CATL, Cosponsored by COMP

Quantum Dynamics in Large Scale Systems

Large-Scale Simulations in Materials Systems

Sponsored by PHYS, Cosponsored by COMP

TUESDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Material Science

Properties

C. M. Aikens, *Organizer*

R. C. Remsing, *Presiding*

1:30 COMP **194.** Breaking badly: DFT-D2 gives sizeable errors for tensile strengths in bulk solids. **B.M. Wong**, N. Ilawe

2:00 COMP **195.** Simulation of shock-wave properties in fused silica using soft-core potential. **S. Izvekov**, E.F. Byrd, N. Weingarten, B.M. Rice

2:30 COMP **196.** Reactive modeling of silica formation. J. Deetz, **R. Faller**

3:00 Intermission.

3:30 COMP **197.** Nanoscale charge balancing mechanism in alkali substituted C-S-H gels from first-principles calculations. **O. Ozcelik**, C. White

4:00 COMP **198.** Impact of environment on mechanical and physical properties of polyethylene: Comparison between experiments and simulation. **A. Shamloo**, A. Soldera, D. Rodrigue

4:30 COMP **199.** Computational studies of crystallization on the nanoscale. **J. Delhommelle**, C. Desgranges

5:00 COMP **200.** Modeling and simulations of functionalized magnetic nanoparticles as drug delivery systems. K. Karathanou, **Z. Cournia**

Section B

InterContinental San Francisco

Fremont

Catalytic Materials from Molecular Insight

Cosponsored by CATL, MPPG‡ and PHYS

K. Honkala, B. Liu, *Organizers*

A. Z. Clayborne, *Presiding*

8:30 COMP **201.** Catalysis by functionalized nanoparticles. **N. Lopez**

9:05 COMP **202.** Computational design of nanoalloy catalysts from DFT, genetic algorithms and machine learning. **T. Vegge**, P.C. Jennings, T. Bligaard, H.A. Hansen

9:40 COMP **203.** Subnanometer metal clusters as catalysts for energy conversion and storage. **L.A. Curtiss**, C. Liu, P. Zapol, S. Vajda

10:15 Intermission.

10:35 COMP **204.** Alloying supported Pt clusters with boron: Coke antagonist. **A. Alexandrova**, M. Ha, E. Jimenez-Izal

11:10 COMP **205.** Revealing the pathway of CO_2 reduction in a multicenter iron carbonyl catalyst using an *ab initio* nanoreactor. **L. Wang**, M.E. Hutchings, Y. Qiu

11:30 COMP **206.** Ab initio study of the hydrogen-producing mechanisms of cobaloximes in acetonitrile-water mixtures. **J. Chen**, P. Sit

11:50 COMP **207.** Protein-environment effect on catalysis performance in H_2-producing [NiFe] hydrogenases. **S. Qiu**, L.M. Azofra, D.R. MacFarlane, C. Sun

Section C

InterContinental San Francisco

Howard

Strong Electron Correlation & Nonadiabatic Dynamics

Cosponsored by PHYS

G. Gidofalvi, E. Hohenstein, *Organizers*

A. E. DePrince, *Organizer, Presiding*

1:30 COMP **208.** Two-electron reduced density matrices in electronic structure and dynamics. **D.A. Mazziotti**

2:10 COMP **209.** Using single-exciton wavefunctions to compute exciton-binding energies in singlet fission materials. **N. Mayhall**

2:40 COMP **210.** Strong correlation in coupled F-centers. **B.G. Janesko**

3:10 Intermission.

3:25 COMP **211.** Quantum chemistry strategies: Addressing strongly correlated transition metal and heavy element species. C. Plascencia, S. Yuwono, G. Schoendorff, **A.K. Wilson**

4:05 COMP **212.** Recent developments with the multifacet graphically contracted function electronic structure method. **R. Shepard**, S.R. Brozell, G. Gidofalvi

4:45 COMP **213.** Multi-reference electron correlation with large active spaces from time-dependent perturbation theory with density matrix renormalization group. **A. Sokolov**, G. Chan

Section D

InterContinental San Francisco

Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

N. J. Deyonker, *Presiding*

1:30 COMP **214.** Atropisomerization of 8-membered dibenzolactam: Experimental NMR and theoretical DFT study. **A. Buevich**

1:55 COMP **215.** Computational study of the photoelectron spectra of Europium-oxide, -hydride, and -hydroxide. **H. Harb**, L.M. Thompson, H.P. Hratchian

2:20 COMP **216.** Reaction mechanism of group II introns hydrolytic splicing investigated by QM/MM MD simulations. **L. Casalino**, G. Palermo, U. Roethlisberger, A. Magistrato

2:45 COMP **217.** Reactive first principles Monte Carlo simulations of nitrogen/oxygen and hydrogen sulfide/carbon dioxide mixtures. **E. Fetisov**, M. Shah, I.W. Kuo, C. Knight, J. Siepmann

3:10 Intermission.

3:25 COMP **218.** Combining quantum and QSAR methods for prediction of acid dissociation constants. L. Hosseini-Gerami, R. Leth, P. Hunt, **M.D. Segall**

3:50 COMP **219.** Computational investigation of o-aminomethylphenylboronic acid saccharide receptors. **J. Larkin**

4:15 COMP **220.** TINKTEP: Polarizable QM/MM based on linear-scaling DFT and the AMOEBA force field. **J. Dziedzic**, M.P. Head-Gordon, T.L. Head-Gordon, C. Skylaris

4:40 COMP **221.** Solvent/enzyme-perturbed transition state sampling and its applications. **Z. Yang**, Y. Li, J. Park, C. Doubleday, K.N. Houk

Section E

InterContinental San Francisco

Laurel Hill

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Cosponsored by BIOL, MEDI and WCC

D. J. Kempf, T. R. Stouch, *Organizers*

Y. C. Martin, *Organizer, Presiding*

1:30 COMP **222.** Collaborating to bring resources to neglected diseases research. **D.J. Kempf**

2:00 COMP **223.** NTD drug discovery booster: A novel approach for hit to lead chemistry. **B. Perry**

2:30 COMP **224.** Combining strengths of phenotype and target-based approaches to discover novel TB drugs. **J. Sacchettini**

3:00 Intermission.

3:15 COMP **225.** Antitubercular 3-(4- aminophenyl)oxazolidin-2-ones: Progress towards better, safer TB agents. **C.B. Cooper**

3:45 COMP **226.** Tylosin analogs as anti-filarial agents: Medicinal chemistry optimization and candidate selection. **T.W. Von Geldern**, D.J. Kempf, K. Marsh, H.E. Morton, L. Ford, J. Turner, S. Ward, M. Taylor, A. Hoerauf, S. Specht

‡ *Cooperative Cosponsorship*

4:15 COMP **227. Award Address** (ACS Award for Computers in Chemical & Pharmaceutical Research sponsored by ACS Division of Computers in Chemistry). CADD and chemoinformatics within an inter-institution collaboration for TB drug discovery. **Y.C. Martin**

Section F

InterContinental San Francisco

Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG‡

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

1:30 COMP **228.** Recent advances in the quantum simulation of materials. **G.E. Scuseria**

1:55 COMP **229.** Making density-functional embedding theory applicable to spin-polarized materials and covalent materials. **C. Huang**, A.B. Munoz, M. Pavone

2:20 COMP **230.** Ab-initio materials spectra. J. McClain, T. Berkelbach, Q. Sun, **G. Chan**

2:45 COMP **231.** Alchemy, chemical space, and quantum mechanics. **O. von Lilienfeld**

3:10 Intermission.

3:30 COMP **232.** Finite-temperature *ab initio* many-body perturbation and coupled-cluster calculations of condensed matter. **S. Hirata**

3:55 COMP **233.** Self-consistent many-body methods for bond-making and breaking. **P. Rinke**

4:20 COMP **234.** Fast and accurate quantum Monte Carlo methods for material science. **D. Alfe**, A. Zen, M. Gillan, S. Sorella, A. Michaelides

4:45 COMP **235.** Extending the applicability of quantum Monte Carlo methods to large molecules. **C. Filippi**

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Electrocatalysis

Sponsored by CATL, Cosponsored by COMP

Quantum Dynamics in Large Scale Systems

Large-Scale Simulations in Biological Systems

Sponsored by PHYS, Cosponsored by COMP

TUESDAY EVENING

Section A

Moscone Center

West Hall

Chemical Computing Group Graduate Student Travel Awards

K. N. Kirschner, C. L. Simmerling, *Organizers*

6:00 - 8:00

COMP **236.** QM-NEW: An efficient and accurate QM/MM free energy estimator and its application to pKa predictions. **F.L. Kearns**, P.S. Hudson, S. Boresch, H.L. Woodcock

COMP **237.** Automatic and systematic construction of active spaces from the atomic valence orbitals. **E.R. Sayfutyarova**, G. Chan

COMP **238.** Controlling coherent electron transfer in bi-nuclear platinum complexes. **P.J. Lestrange**, D.B. Lingerfelt, X. Li, L.X. Chen

COMP **239.** Molecular simulations provide crucial insights into the mechanisms of biocatalysis in ionic liquids. **K. Sprenger**, J. Pfaendtner

Section B

Moscone Center

West Hall

COMP Poster Session

H. L. Woodcock, *Organizer*

6:00 - 8:00

COMP **240.** Investigating the fluorescence mechanism of boron-nitrogen based glucose chemosensors and non-traditional hydrogen bonding in B_2H_6 -benzene complexes. **F.L. Kearns**, C. Robart, M.T. Kemp, J. Larkin, H.L. Woodcock

COMP **241.** New approach for detection and visualization of aggregation-prone regions. **C. Williams**

COMP **242.** Microsecond molecular dynamic simulations on the second hydride transfer transition state of *Pseudomonas mevalonii* 3-hydroxy-3-methylglutaryl reductase using Q2MM. **T. Quinn**, B.E. Haines, J. Lei, H. Jiang, X. Huang, P. Helquist, O. Wiest

COMP **243.** Benchmarking excited state absorption via LR/RT-TDDFT for a series of organic chromophores. **J. Asher**, D.N. Bowman, N. Govind, C.J. Cramer

COMP **244.** Steric effects in the computational modeling of enediynone cyclization reactions. **K. Hoang**, C.Q. Li, B.F. Gherman, J.D. Spence

COMP **245.** Hydricity calculation of catalysts using DFT methods. **H. Fallah**, K.R. Brereton, A.J. Miller, T.R. Cundari

COMP **246.** Modeling 10000 antibodies in about an hour: Leveraging the power of the Amazon Cloud. **E. Metwally**

COMP **247.** Improving drug design by predicting exposed polarity. **F. Ruggiu**, B. Shirley, J.M. Jansen, H.E. Moser

COMP **248.** Prediction of API oxidative liability: *In silico* approach towards antioxidant selection, a collaboration of the Medicinal Chemistry, Formulation Sciences and DMPK departments at AbbVie. **H. Geneste**, L. Asmus, G. Backfisch, M. Degenhardt, F. Oellien

COMP **249.** Design of novel inhibitors for the aldehyde dehydrogenases. **E. Selner**, **C. Magee**, L.W. Peterson, M.L. Cafiero

COMP **250.** DFT analysis of the selectivity of known bioactive ligands in the sulfotransferase and catechol-o-methyltransferase enzymes. **C. Pinckney**, C. Magee, L.W. Peterson, M.L. Cafiero

COMP **251.** Towards more accurate models of organic electro-optic materials: Computing the hyperpolarizabilities of dimer and tetramer charge-transfer chromophores. **J. Maat**, C. Isborn, X. Sosa Vazquez

COMP **252.** Design and synthesis of novel inhibitors for the tyrosine hydroxylase enzyme. **R. Evans**, L.W. Peterson, M.L. Cafiero

COMP **253.** Analysis of random alloy nanoparticles as catalysts for oxidation reduction reactions. **F. Al-Quaiti**, J. Duncan, B. Corona, C. Lee, E. Trevino, G.A. Henkelman

COMP **254.** Exponential relationships capturing atomistic short-range repulsion from the Interacting Quantum Atoms (IQA) method. **A. Wilson**, P. Popelier

COMP **255.** Withdrawn.

COMP **256.** Machine-learning-assisted characterization of chemical transitions: Inhomogeneous mechanisms underlying reactions in homogeneous solution. **J. Zhang**, Z. Zhang, Y. Gao

COMP **257.** Computational outlook on ferroelectricity: Transition state optimizations and charge analysis. **M. Romero**, D. Miller, E. Zurek

COMP **258.** New approaches to the computational chemistry and computer-assisted application of calculation for steroids. E.J. Parish, G. Ren, Y. Lo, **M. Hsiao**, **H. Honda**, T. Wei

COMP **259.** Novel application of mathematical model to the development of biosensor for high blood cholesterol. **G. Ren**, Y. Lo, **H. Honda**, E.J. Parish

COMP **260.** Interplay between crystallization and glass transition in bimetallic nanoalloys. **S. Bechelli**, C. Desgranges, J. Delhommelle

COMP **261.** Molecular simulation of gas adsorption in metal-organic frameworks. **G. Karuppasamy**, C. Desgranges, J. Delhommelle

COMP **262.** Nitrogen-doped graphene nanoflakes: Electronic and optical properties depending on flake sizes and dopant positions. **C. Lin**

COMP **263.** Hydrogen placement on potential organic ferroelectric NUBHOH. **M. Ynfante-Corral**

COMP **264.** Activity coefficients of sodium chloride (NaCl) at varying concentrations and temperatures calculated using molecular dynamics simulations. **A. Kasinski**, P.B. Moore, R.L. Napoleon

COMP **265.** Investigating the hydration of polyamide 6 using theoretical difference infrared spectroscopy. **B. Thomsen**, Y. Sugita, K. Yagi

COMP **266.** Simulating the binding pathways of sialic acid and oseltamivir to H274Y neuraminidase with molecular dynamics simulations. **D.F. Dacres**, E.M. Lewis, R. Wenner, A.W. Van Wynsberghe

COMP **267.** Polypeptide bonding to surface studied by computational analysis of x-ray photoelectron spectra. **I. Tolbatov**, D. Chipman

COMP **268.** Solvation free energies via alchemical free energy calculations: Applications and challenges. **G. Duarte Ramos Matos**, D.Y. Kyud, G. Calabrò, D.L. Mobley

COMP **269.** Mechanistic analysis of a palladium-catalyzed enantioselective decarboxylative allylic alkylation reaction. **A. Sargent**, A.T. Morehead

COMP **270.** Computing aqueous absorption spectra: Effect of solute polarity and basis set on convergence with respect to the amount of explicit solvent. **J. Milanese**, C. Isborn

COMP **271.** Ionization potential optimized hybrid exchange-correlation functional: Improving the accuracy of both core excitation energies and ground state properties. **Y. Jin**, R.J. Bartlett

COMP **272.** Localizing frustration in proteins using coevolutionary information. **B. Sirovetz**

COMP **273.** Ab initio molecular dynamics simulations, reaction energy profiles and reaction rates constants expressions relevant to Titan's atmosphere: CH + C_2H_2 and H + CH_2CCH_2. **X. Torres-Garcia**, J.M. Lopez-Encarnacion

COMP **274.** Divergent mechanistic pathways in a metal-catalyzed hydroacylation reaction. **E. Bolger**, A.T. Morehead, A. Sargent

COMP **275.** DFT, CCSD and CASSCF investigations of 1,1 elimination transition state geometries and post-transition state complexes of hydrofluorocarbons. **M. Nestler**, G.L. Heard, B.E. Holmes

COMP **276.** Vanddraabe: Identification and statistical analysis of structurally conserved waters via R. **E.X. Esposito**

COMP **277.** Plunger method for simulating polymer crystal-melt interfacial tensions. **Q. Chen**, D. Kozuch, S. Milner

COMP **278.** Fullerene based materials for cathodic applications in lithium ion battery. **P. Sood**, K. Kim, S.S. Jang

COMP **279.** Towards understanding the chemical physics of the spinach fluorogenic RNA aptamer. **K. Range**, I. Bieker, D.M. York

COMP **280.** Molecular dynamics simulation study of Normetanephrine (NMN) on amyloid-beta 40 monomer aggregation for treatment of Alzheimer's disease. **K. Shim**, J. Kim, C. Shin, J.R. Kim, S.S. Jang

COMP **281.** Analysis of the role of the electronic structure on lithium diffusion in Li10GP2S12 and -Li3PS4 solid electrolytes. **A.T. Hall**, N. Leclerc, N. Adelstein

COMP **282.** Novel approaches to the bioinformatics application of spreading factor in the domain identification and functional prediction. Y. Lo, **G. Ren**, H. Shyu, **H. Honda**, T. Wei

COMP **283.** Density functional solution for nondynamic and strong correlation. **J. Kong**, E. Proynov, F. Liu

COMP **284.** Automating isotope effects computations and analyses. A. Brueckner, S. Cevallos, **O. Ogba**, D.J. O'Leary, P. Cheong

COMP **285.** Atomic-scale simulations of self-assembling peptide-conducting polymer hybrid materials. **H. Pan**, Z. Pollard, E. James, A. Murphy, T. Kowalczyk

COMP **286.** Color-based illustration of the maximum overlap method. **Z. Pollard**, K. Le, T. Kowalczyk

COMP **287.** Accurate estimate of ligand-binding affinity using alchemical free energy calculation via metadynamics. **Y. Tanida**, A. Matsuura

COMP **288.** Modeling rhodium-catalyzed hydroacylation of formylstyrene: Competitive formation of indanone and tetralone products. **T. Shoopman**, A.T. Morehead, A. Sargent

COMP **289.** Transition state of a 17 minute timescale drug unbinding event. **S. Lotz**, A. Dickson

COMP **290.** Visualization of convolutional neural network scoring of protein-ligand binding. **J. Hochuli**, M. Ragoza, D. Koes

COMP **291.** Auto generation of Markush structure for maximizing composition patent claim. **P. Wang**, **Y. Tseng**

COMP **292.** Putting electrostatics and water at the center of structure-based drug design. **T. Cheeseright**, M.D. Mackey, G. Tedesco, P. Tosco, S. Tomasio

COMP **293.** Understanding the behaviour of multifunctional gold nanoparticles (AuNPs). **A. Raman**, C. Jaime, V.F. Puntes

COMP **294.** Effect of ethanol infiltration into dentin collagen fibrils using molecular dynamics simulation. **J. Liu**, **S. Davis**, H. Du, E. Cho, Z. Abrams, M. Lee, J. No, S. Jee, S.S. Jang

COMP **295.** Novel Zn binding moiety for LpxC identified by data mining, virtual screening, and experimental validation. **P.S. Lee**, C. Bellamacina, J. Bojkovic, Z.K. Sweeney, J. Fu, L. Xie, W. Shu, K. Uehara, L. McDowell, A. Lingel

COMP **296.** Impact of sequence homology on DNA microarray hybridization interactions: A Monte Carlo molecular simulation study. K.J. Mei, C. Lucy, M. Pham, **J.M. Stubbs**

COMP **297.** Investigation of rhodium catalysts and reactants for hydroacylation reactions. **E. Schneider**, J. Scanlon

COMP **298.** Sulfur bonds: Exploration of a novel non-covalent intermolecular bond and its role in drug development. **M.R. Koebel**, G. Schmadeke, S. Sirimulla

COMP **299.** Mixed reality visualization application for drug discovery research. **G. Uranga**, S. Sirimulla

COMP **300.** Connectivity-based hierarchy to eliminate systematic errors: Accurate combustion properties of biofuel molecules using DFT. **S. Debnath**

COMP **301.** Molecular dynamics simulation of the behavior of copper atoms in hydrated zeolite Cu-SSZ-13. **D. Clavijo Gutierrez**, A. Chaparro, E. Jaramillo

COMP **302.** Quantum mechanical calculations of UV-VIS spectra of conjugated molecules. **I. Bieker**, B. May

COMP **303.** Synthesis and structure prediction of a novel, potentially electroactive, organic material. **S. Jacinto**, K.R. Cousins, T. Usher

COMP **304.** Ab initio characterization of halogen bonds involving molecular ionic halogen bond donors. K. Tran, **K. Riley**

COMP **305.** CMDnavigator: A tool for interactive analysis and visualization of peptide data. **A.S. Bayden**, D.J. Diller, J.H. Audie, K. Diller

COMP **306.** Spatially extended active sites: Building favorable electrostatic interactions in natural and designed enzymes. T.A. Coulther, P.J. Beuning, **M.J. Ondrechen**

COMP **307.** Mixed lithium indium halides as solid-electrolytes: Computational experiments on drivers of Li^+ diffusion. **T.C. Alves**, A. Zevgolis, **N. Adelstein**

COMP **308.** Identification of promiscuous enzymes for the aza-Morita-Baylis-Hillman reaction. **K. Ozturk**, S. Sayin, N. Celebi-Olcum

COMP **309.** Estimating kinetic rates for β-cyclodextrin. **H. Pratt**, B.R. Jagger, C. Lee, R.E. Amaro

COMP **310.** Conformational dynamics of histone lysine methyltransferases by millisecond-timescale molecular dynamics on Folding@home. **R.P. Wiewiora**, S. Chen, K. Beauchamp, M. Luo, J.D. Chodera

COMP **311.** Multiscale estimation of kinetic rates of trypsin with benzamidine using a hybrid molecular dynamics, brownian dynamics, and milestoning approach. **B.R. Jagger**, L. Votapka, A. Heyneman, R.E. Amaro

COMP **312.** Prediction of pH dependent NMR chemical shifts. **E. Artikis**, C.L. Brooks

COMP **313.** Generic interface streamlines access to results from expertly prepared 3D models. **T. Mansley**, E. Champness, C. Leeding, P. Hunt, N. Foster, M. Segall

COMP **314.** Computational studies of electrochemical initiation of reactions involving nitrogen-radical precursors. **S. Calderon**, H.P. Hratchian

COMP **315.** Bond dissociation enthalpies of halomethanes, haloethanes, haloethenes, and haloacetylene. **K.R. Jorgensen**

COMP **316.** Photocatalytic and electronic implications from first principles characterization of oxygen depletion localized on TiO_2 brookite nanoparticle surfaces. **K.G. Johnson**, E.A. Jarvis

COMP **317.** *Ab initio* characterization of intramolecular and energetic features of the water oxidation mechanism for mononuclear ruthenium and iron catalysts. **K. Hunter**, E.A. Jarvis

COMP **318.** Computational study of how β-loop dynamics regulate HCV polymerase activity in the presence and absence of thumb-site-II inhibitors. **N. Ibrahim**, J. Li, K. Johnson, S. Kirmizialtin

COMP **319.** DFT design of inhibitors of the LpxC enzyme. **C. Dishuck**, R. Roldan, A.J. Dewar, L.W. Peterson, M.L. Cafiero

COMP **320.** DFT study of the selectivity of phenylalanine hydroxylase. **M.C. Perchik**, L.W. Peterson, M.L. Cafiero

COMP **321.** Modeling excited states of the OH radical reaction with cyclopentadiene and the cyclopentadienyl radical. **P.B. Orndorff**, J.B. Foresman

COMP **322.** DFT study of the selectivity of the tyrosinase active site. **D. Wilson**, S. Fields, L.W. Peterson, M.L. Cafiero

COMP **323.** Linkage isomerization In phosphine substitution reactions of $CpRu(PPh_3)_2NCS$. **D. Dang**, R.U. Kirss

COMP **324.** DFT study of the selectivity of monoamine oxidase B (MAOB). **S. Jelinek**, M. Morris, L.W. Peterson, M.L. Cafiero

COMP **325.** Structural insights of a PI3K/mTOR dual inhibitor with the morpholino-triazine scaffold. **T. Takeda**, Y. Wang, S.H. Bryant

COMP **326.** Effect of Gly to Ser mutations at the integrin-binding site on type I collagen. **A. Mekkat**, H. Yu, B. Brodsky, Y. Lin

COMP **327.** Mechanism for the stereoselectivity in metal-salen catalyzed electroreductive cyclization reactions. **L. Bellini**, M.N. Cihak, B.E. Silva, B.F. Gherman, J.A. Miranda

COMP **328.** Withdrawn.

COMP **329.** Approach for analyzing protein pockets using properly interacting probe molecules. **H. Sato**, A. Matsuura

COMP **330.** Elucidating the mechanism of protein unfolding and translocation by the ClpY ATPase during protein degradation. **Y. Shih**, G. Stan

COMP **331.** Quantum mechanical investigation of the inner sphere reduction mechanism of the [(NSNSN)Co(III)Cl^+] and [(NSSSN)Co(III)Cl^+] cations by iron(II). **W. Smith**, T.A. Jackman, O. Sode

COMP **332.** Molecular simulation of transport of DNA grafted nanoparticles. **S. Ciobotarescu**, J. McLaughlin, C. Desgranges, J. Delhommelle

COMP **333.** Molecular simulations of bubble formation in metastable liquids. **B. Gonzalez**, L. Huber, C. Desgranges, J. Delhommelle

COMP **334.** Subset system study of diisopropylammonium bromide: An organic ferroelectric crystal. **C.M. Sanchez**

COMP **335.** Investigation of different binding kinetics among the neuraminidase inhibitors. **G. Kang**, A.W. Van Wynsberghe

COMP **336.** Examining the binding pathways of peramivir to wild-type neuraminidase through molecular dynamics simulations and MM/GBSA analysis. **R. Wenner**, A.W. Abera, B.J. Banman, A.W. Van Wynsberghe

COMP **337.** DFT study of the selectivity of DOPA-decarboxylase. **E. Harrison**, A.R. Ritter, L.W. Peterson, M.L. Cafiero

COMP **338.** Modeling material properties and charge transfer for lithium-ion batteries. **L. Raguette**, R. Jorn

COMP **339.** Analysis of MM/GBSA free energy calculations to investigate the binding pathways of neuraminidase. **E.M. Lewis**, P.F. Marris, L.M. Krause, A.W. Van Wynsberghe

COMP **340.** Novel approaches to the computer assisted informatics of oxysterol and 7-ketocholesteryl benzoate. E.J. Parish, **G. Ren**, Y. Lo, **H. Honda**

COMP **341.** Automated selection of active orbital spaces. **C.J. Stein**, M. Reiher

COMP **342.** Computational studies of the UV/visible absorption spectra of selected merocyanine dyes. **I. Tolbatov**, S. Grimme

COMP **343.** Examining ligand recognition in RNA aptamers via molecular dynamics simulations. **P. Gasper**, A.A. Chen

COMP **344.** Development of a coarse-grained model of polypeptoids for studying self-assembly in solution. **P. Du**, R. Kumar

COMP **345.** Fragment ER: Efficient and accurate binding free energy calculation method for protein-ligand complex. **T. Masuda**, R. Tanimura, N. Matubayasi

COMP **346.** Accurate absorption spectra of aqueous estrogen derivatives via molecular dynamics/EOM-CCSD. **D. Ruuska**, M. Paul, S.N. Eustis

COMP **347.** Visualising the molecular drivers behind drug resistance. **M. Malaisree**, C.J. Woods

COMP **348.** Predicting polythiophene electronic structures: Statistical model screening for the efficient discovery of OPV materials. **M. Cole**, I. Kanal, G. Hutchison

COMP **349.** Molecular simulation study of the 3,4-dihydroxymandelic acid on amyloid beta 40 monomer for treatment of Alzheimer's disease. **E. Tumurbaatar**, J. Kim, C. Shin, S. Jang, J.R. Kim

COMP **350.** Modelling UV-vis spectra for a series of alkenyl substituted pyrroles. **R. Fair**

COMP **351.** Computationally predicted signatures of EGFR exon 20 insertions in non small cell lung cancer and its response to irreversible inhibitors. **B. Su**, D. Huang, P. Wang, O. Lin, **Y. Tseng**

COMP **352.** Longtime simulation of dynamical fractures in vault nanoparticles through multiscale molecular dynamics. **J.M. Espinosa Duran**, A. Abi Mansour, P. Ortoleva

COMP **353.** Molecular modeling of small molecule inhibitors of the Hv1 proton channel. **V.T. Lim**, A.D. Geragotelis, N. Lim, J.A. Freites, D.L. Mobley, D. Tobias

COMP **354.** *In silico* measurements of the ionic current in a K^+ ion channel using weighted ensemble simulations. **S. Capponi**, H. Siddiqi, J. Adelman, J. Rosenberg, M. Grabe

COMP **355.** Ligand- and receptor-based virtual screening for inhibitors of the signal transducer and activator of transcription 5 (STAT5). **E. Gianti**, G. Fiorin, M.L. Klein, R.J. Zauhar

COMP **356.** Incorporating continuum solvent-based receptor desolvation into molecular docking. **R. Stein**, T.E. Balius, B. Shoichet

COMP **357.** Evaluating use of tens to hundreds of active ligands in pharmacophore hypothesis perception. **E.T. Mack**, S.L. Dixon, C.D. Von Bargen, M.P. Repasky

COMP **358.** Density functional theory study of the binding of tyrosine and phenylalanine with graphene. **D.A. Daggag**, J. Lazare, T. Dinadayalane

COMP **359.** Molecular modeling of multicompartment micelle nanoreactors. **C.P. Callaway**, P. Sood, S. Jang

COMP **360.** Identification of ZIKA virus inhibitors using insilico screening. **M. Rivera**, S. Sirimulla

COMP **361.** Non-adiabatic QM/MM: A hybrid approach to doing non-adiabatic excited state dynamics. **D.A. Tracy**, J. Bjorgaard, S. Tretiak, A.E. Roitberg

COMP **362.** Rationalization and visualization of non-bonded interactions using extended Hückel theory. A. Ajamian, C. Williams, P. Labute, **N. Li**

COMP **363.** Simulations of small molecule diffusion in polyelectrolyte solutions. **P.K. Walhout**, Z. He, A.A. McMillan, T.D. Sedlacek

COMP **364.** Python program for solving problems in computer-aided peptide design. **A.S. Bayden**, J.H. Audie, D.J. Diller

COMP **365.** Effects of virion structural changes on binding events related to molecular mechanisms of influenza infections by brownian dynamics simulations. **S.E. Kochanek**, J.D. Durrant, R.E. Amaro

COMP **366.** IKKβ dynamic structure regulates NF-κB pathway in inflammatory response. **T.T. Nguyen**, J. Schiffer, G. Ghosh, R.E. Amaro

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

COMP **367.** Engineering increased activity into a ketosteroid isomerase homologue through predictive computational methods. **G. Levine**, T.A. Coulther, P.J. Beuning, M.J. Ondrechen

COMP **368.** Information-driven fully flexible HADDOCKing: Performance on a benchmark of protein-ligand complexes. **J. Grinstead**, A. Thureau, J.P. Rodrigues, K.R. Reinke, A.F. Ramsing, T.L. Wormwood, A. Bonvin

COMP **369.** Docking studies of camodulin and fulvic acid. **F.C. Zhang**, L. Liu, Y. Wu

COMP **370.** First-principles study of di-substituted donor moieties on NLO properties: Theoretical paradigms of interactive computation. **M. Janjua**

COMP **371.** Study on the interaction between resveratrol and CopC by spectroscopic and docking methods. Z. Song, **F.C. Zhang**

COMP **372.** $C_{59}Pd$: A novel heterogeneous catalytic material for Suzuki-Miyaura reaction. **M.C. Padole**, P. Deshpande

COMP **373.** Withdrawn.

COMP **374.** PYCED: An efficient technique to simulate charge and exciton dynamics coupled with DFT methods for large systems. **P. Ramos**, M. Pavanello

COMP **375.** Theoretical investigation of electron-nuclear dynamics in the $[Au_{25}(SH)_{18}]^{-1}$ thiolate-protected gold nanocluster. **R.D. Senanayake**, A.V. Akimov, C.M. Aikens

COMP **376.** Withdrawn.

COMP **377.** Predicting *N*-methylated cyclic peptide structures to inform force field development. **D. Slough**, H. Yu, S. McHugh, Y. Lin

COMP **378.** ALKBH7 variant related to prostate cancer exhibits altered substrate binding. **A. Walker**, P. Silvestrov, T.A. Müller, R.H. Podolski, G. Dyson, R.P. Hausinger, G.A. Cisneros

COMP **379.** Withdrawn.

COMP **380.** Supramolecular effects in radical chemistry. **G. Gomes**, I. Alabugin

COMP **381.** Withdrawn.

COMP **382.** *In silico* discovery of high performance organic polymers for optical applications. **M. Afzal**, J. Hachmann, C. Cheng

COMP **383.** Linear absorption spectra from explicitly time-dependent equation-of-motion coupled-cluster theory. **D.R. Nascimento**, A.E. DePrince

COMP **384.** Withdrawn.

COMP **385.** Plasmonic resonances: A systematic analysis of metallic nanoparticles using real-time, time-dependent DFTB. **N. Ilawe**

COMP **386.** Withdrawn.

COMP **387.** Kirkwood Buff derived force field for some biologically important oxo anions. **N. Naleem**, P.E. Smith

COMP **388.** Withdrawn.

COMP **389.** Scaffold repurposing of ring-constrained nucleosides: A molecular modeling perspective. **A. Ciancetta**, D. Tosh, K.A. Jacobson

COMP **390.** Systematic parameterization of lignin for the CHARMM force field. **J.V. Vermaas**, L. Petridis, G. Beckham, M.F. Crowley

COMP **391.** Elucidating the functional roles of spatial organization in cross-membrane signal transduction by a hybrid simulation method. **Y. Wu**

COMP **392.** Insights into the nature of glass formation from ultra-efficient simulations of the supercooled state. **D.S. Simmons**, J. Hung, T.K. Patra, J. Mangalara, V. Meenakshisundaram

COMP **393.** Toward polarizable AMOEBA thermodynamics at fixed charge efficiency using a dual force field approach: Application to peptides and proteins. J.M. Litman, S.D. LuCore, C. O'Connell, **M.J. Schnieders**

COMP **394.** Understand protein functions by comparing the similarity of local structural environments. **Y. Wu**

COMP **395.** Large-scale v2RDM-driven CASSCF methods. **A.E. DePrince**

COMP **396.** Ligand residence times from simulation using loosely coupled parallel trajectories. **A. Dickson**

COMP **397.** Elucidating mechanisms of RNA recognition and processing in the exosome complex via enhanced sampling molecular dynamics simulations. **L. Vukovic**

COMP **398.** Incorporation of sigma hole scoring function in Autodock Vina. **S. Sirimulla**

COMP **399.** Hard-sphere Monte Carlo model of nanomaterial toxicity. **N. Assefa**

COMP **400.** Investigating the structure of PEI-nucleic acid gene delivery complexes using molecular dynamic simulations. **N. Walker**

COMP **401.** Elucidating binding mechanisms of ABA analogues: Activation of PYL5 receptor by pyrabactin and quinabactin. **M. Meigooni**, C. Zhao, D. Shukla

COMP **402.** Binding site protonation and self-correcting occlusion control the Na^+/K^+-pump selectivity. **H. Rui**, P. Artigas, B. Roux

COMP **403.** Towards a rational design of macrolide antibiotics in order to combat the bacterial resistance. **A. Pavlova**, J.M. Parks, A.K. Oyelere, J. Gumbart

COMP **404.** Physiologically relevant transmembrane potential modelling of complex lipid bilayer systems. **X. Lin**, A. Gorfe

COMP **405.** Interaction affinity of biological molecules with 2D materials. **N. Saikia**, K. Waters, U. Saikia, M. Seel, R. Pandey

COMP **406.** Comparative analysis of the structural determinants of endogenous cannabinoids and activity of illicit drugs on cannabinoid receptors. **V.K. Yadav**, K.M. Elokely, M.L. Klein

COMP **407.** Catalytic mechanism of RNase A transphosphorylation. **M. Huang**, D.M. York

COMP **408.** Implementation of analytic gradient for FMO RI-MP2 method. **B.Q. Pham**, M.S. Gordon

COMP **409.** Modeling and simulation of AcrB multi drug transporters functional dynamics. **S. Jamshidi**, M. Sutton, K.M. Rahman

COMP **410.** Through-space and through-bond stabilization of cis alkenyl anions. **H. Villegas**, K.B. Wiberg, B.G. Janesko

COMP **411.** Community participation in the D3R Continuous Evaluation of Ligand Pose Prediction (CELPP) competition. **J. Wagner**, S. Liu, S.M. Gathiaka, R. Malmstrom, M.K. Gilson, R.E. Amaro

COMP **412.** Simulation of the interaction between polymer-encapsulated air microbubble and blood cell in the blood vessel. **Z. Wang**

COMP **413.** Unified framework for computer-aided biologics design. **A. Deschenes**

COMP **414.** Challenges in the discovery of macrocyclic cyclophilin inhibitors. **U. Schmitz**, D. Shivakumar

Section C

Moscone Center
West Hall

NVIDIA GPU Award

M. E. Berger, C. L. Simmerling, *Organizers*

6:00 - 8:00

COMP **415.** Multiscale modeling of poly(ethylene oxide) with ionic liquids: GPU enabled first-principles force fields. **C. Son**, J. McDaniel, J.R. Schmidt, Q. Cui, A. Yethiraj

COMP **416.** GPU implementation of molecular docking with applications to receptor flexibility and energy landscape sampling. **J. Sunseri**, D. Koes

COMP **417.** Calculation of host-guest binding free energies via the AMOEBA polarizable force field. **M.L. Laury**, J.W. Ponder

COMP **418.** ANAKIN-ME: Using deep learning to develop a fully-transferable and chemically accurate GPU-accelerated potential. **J.S. Smith**, O. Isayev, A.E. Roitberg

COMP **419.** GPU-enabled real-time electron dynamics of nitrogen-doped graphene nanoflakes. **S.I. Allec**, B.M. Wong

Section D

Moscone Center
West Hall

OpenEye Outstanding Junior Faculty Award

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **420.** Multiscale simulations to elucidate enzymatic processing of DNA and RNA. **M. De Vivo**

COMP **421.** Accounting for water in early stage drug discovery and design. **T.P. Kurtzman**

COMP **422.** Accelerating real-time electron dynamics calculations of large plasmonic systems. **B.M. Wong**

COMP **423.** Multireference quantum chemistry and conical intersections at the nanoscale. **B.G. Levine**

COMP **424.** Elucidating heterogeneous ice nucleation mechanisms using large scale rare event simulations. **S. Sarupria**, B. Glatz, R. Defever, W. Hanger, L. Ngo, A. Apon

Section E

Moscone Center
West Hall

Wiley Computers in Chemistry Outstanding Postdoc Award

C. L. Simmerling, *Organizer*

6:00 - 8:00

COMP **425.** Electronic transitions in the condensed phase: Real-time and linear-response time-dependent density functional theory. **M. Provorse**, C. Isborn

COMP **426.** Phospholipases A_2 a pharmaceutical target to diminish inflammation. **V. Mouchlis**, J. McCammon, E.A. Dennis

WEDNESDAY MORNING

Section A

InterContinental San Francisco
Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Cosponsored by PHYS

G. Verkhivker, *Organizer*

C. Chang, *Organizer, Presiding*

8:30 COMP **427.** Allostery through the lens of a computational microscope. **R.E. Amaro**

9:00 COMP **428.** Discrete molecular dynamics approach to the study of protein confrormational changes. **M. Orozco**

9:30 COMP **429.** Molecular simulations of membrane sensing and remodeling dynamics. **G. Hummer**, R. Covino, A. Bahrami, R. Bhaskara, J. Köfinger

10:00 Intermission.

10:20 COMP **430.** ATP hydrolysis as a driver of conformational change, an example of GroEL. J. Liu, K. Kavran, Y. Wang, K. Jia, **R.L. Jernigan**

10:50 COMP **431.** Conformational transition in kinase from explicit solvent simulations and Markov model analysis. **Q. Cui**

11:20 COMP **432.** Surveying key residues for protein allostery using rigid residue scan method. **P. Tao**

Section B

InterContinental San Francisco
Fremont

Material Science

Organic

C. M. Aikens, *Organizer*

A. Abbaspour Tamijani, *Presiding*

8:30 COMP **433.** Functional group dependent conductance of stilbene: A first-principle transport study. **M.R. Neupane**, C. Carlin, C.B. Rinderspacher, J. Andzelm

9:00 COMP **434.** Design principles for organic photovoltaic materials from ab initio simulations. **M.B. Goldey**, D. Reid, J.J. De Pablo, G.A. Galli

9:30 COMP **435.** DFT evidence of unforeseen bending in linearly fused polycyclic rings of hexasilabenzenoids. **A. Gupta**, J. Arora

10:00 Intermission.

10:30 COMP **436.** Identification of next-generation materials for organic solar cells via a collaborative theory-experimental approach. **S.A. Lopez**, N.C. Davy, A. Oh, A. Aspuru-Guzik, Y. Loo

11:00 COMP **437.** Theory linked with experiment in discovering new functional organic/organometallic materials. **K.R. Cousins**, T. Usher, R. Zhang, D. Miller, D.C. Smith

11:30 COMP **438.** Capturing the role of temperature in crystal polymorph stability using molecular modeling. E. Dybeck, N. Abraham, N.P. Schieber, **M.R. Shirts**

12:00 COMP **439.** Predicting relative polymorph stability using multistate reweighting methods and Jacobian mapping. **N.P. Schieber**, E. Dybeck, M.R. Shirts

Section C

InterContinental San Francisco

Howard

Drug Design

Structure-Based Approaches

M. R. Landon, Y. Tseng, *Organizers*

C. Dickson, *Presiding*

8:30 COMP **440.** Structural insight into sodium-dependent sugar transporters and their inhibition mechanism. **P. Bisignano**, C. Ghezzi, A. Paz, C. Kalyanaraman, M.P. Jacobson, R. Friemann, J. Abramson, E. Wright, M. Grabe

8:55 COMP **441.** Structural insight into KRAS A146 mutations from molecular simulations. **T. Abramyan**, K. Rossman, D. Kireev

9:20 COMP **442.** Interdependence of inhibitor recognition in HIV-1 protease subsites. **J.L. Paulsen**, F. Leidner, D. Ragland, N. Kurt Yilmaz, C.A. Schiffer

9:45 Intermission.

10:05 COMP **443.** Systematic investigation of increased protein flexibility in protein-ligand docking with mixed-resolution Monte Carlo. **J.M. Spiriti**, D.M. Zuckerman

10:30 COMP **444.** Computational investigation of the DNA binding domain of p53: A drive towards novel therapeutics. **J.W. Essex**, M.P. Criddle, Z. Ouaray, C. Verma

10:55 COMP **445.** Origin of preferential binding of aryl chloride groups in serine protease S1 pockets: An application of Fragment Symmetry-Adapted Perturbation Theory (F-SAPT) to drug protein binding. **D.L. Cheney**, D.F. Sitkoff, R.M. Parrish, C. Sherrill

11:20 COMP **446.** Dealing with x-ray data in structure-based design: Estimating and visualizing electron density support. A. Meyder, E. Nittinger, G. Lange, R. Klein, **M. Rarey**

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Section D

InterContinental San Francisco

Cathedral Hill

Molecular Mechanics

Foldamers, Carbohydrates, Macrocycles & Cyclic Peptides

M. Feig, *Organizer*

J. F. Rudzinski, *Presiding*

8:30 COMP **447.** Computational investigations of functional arylamide foldamers. **V. Pophristic**, Z. Liu, A. Abramyan, S. Makeneni

9:00 COMP **448.** Mutations tuning the structure and dynamics of amylin fibrils. **F. Tofoleanu**, Y. Yuan, B. Brooks, N. Buchete

9:30 COMP **449.** Molecular dynamics modeling of fluorescent rosette nanotubes. **A. Gonzales**, B. Legesse, T. Yamazaki, H. Fenniri

9:55 Intermission.

10:10 COMP **450.** Developing enhanced sampling methods for cyclic peptides. **S. McHugh**, J. Rogers, H. Yu, Y. Lin

10:35 COMP **451.** Cyclization, docking, and sampling macrocycles with prime. **D.J. Sindhikara**, T. Day, K. Borrelli

11:05 COMP **452.** Seeing the invisible: Dynamics of glycans on neuronal NMDA receptors. **A. Sinitskiy**, N. Stanley, V.S. Pande

11:35 COMP **453.** Revealing the *T. reesei* Cel6A hydrolysis mechanism via transition path sampling. **H. Mayes**

Section E

InterContinental San Francisco

Laurel Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

D. Nascimento, *Presiding*

8:30 COMP **454.** Intersystem crossings kinetics in complex systems: Implementation of minimum energy crossing point search within the fragment molecular orbital method. **D.S. Kaliakin**, Y. Alexeev, D.G. Fedorov, S.A. Varganov

8:55 COMP **455.** One- and three-electron bonding in conjugated hydrocarbons. **M. Alkan**, A. Rogachev

9:20 COMP **456.** Nonadiabatic molecular dynamics with delta-SCF excited states. **A.V. Akimov**

9:45 COMP **457.** Nonadiabatic transition state theory: Application to intersystem crossing in Cl_2CS. **A.O. Lykhin**, S.A. Varganov

10:10 Intermission.

10:25 COMP **458.** Electronic structure of single molecule magnets. **B. Vlaisavljevich**, D.E. Freedman, S.T. Liddle, L. Gagliardi, T. Shiozaki

11:00 COMP **459.** Computational study of metal-oxo reactive species in porous media with strongly correlated methods. **K.D. Vogiatzis**, L. Gagliardi, E. Pidko

11:35 COMP **460.** Modelling the pump-probe spectroscopy of opsin mimics. **B. Demoulin**, G. Cerullo, I. Rivalta, M. Garavelli

Section F

InterContinental San Francisco

Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG‡

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

8:30 COMP **461.** Calculations of NMR shifts in metallic and insulating solids. **P. Blaha**

8:55 COMP **462.** Computational studies of metal oxide clusters as models for surface defect sites: Modeling electron detachment with efficient electronic structure methods. **H.P. Hratchian**

9:20 COMP **463.** Nonlinear properties from TDDFT: Trials and tribulations. **S.M. Parker**, F.U. Furche

9:45 COMP **464.** Scalable all-electron theory of real-world molecules and materials - examples: Light harvesting and NMR. **V. Blum**

10:10 Intermission.

10:30 COMP **465.** Functional 2D and 3D borides. P.J. Robinson, Z. Cui, **A. Alexandrova**

10:55 COMP **466.** Challenges in calculating the bandgap of triazine-based carbon nitride structures. **S.N. Steinmann**, S. Melissen, T. Le Bahers, P. Sautet

11:10 COMP **467.** Optical properties of highly absorbing Helquat derivatives: *Ab initio* study. **D. Galaktionova**, E. Muchová, P. Slavicek

11:25 COMP **468.** Finding intersystem crossing points between two single-reference potential energy surfaces. **X. Sheng**, L.M. Thompson, H.P. Hratchian

11:40 COMP **469.** Describing a strongly correlated model material system with a mean-field method. **J. Kong**, E. Proynov, J. Yu, R. Pachter

12:05 COMP **470.** *Ab initio* modeling of charge transport defects in quantum dot arrays. **M.B. Goldey**, N.P. Brawand, M. Voros, G.A. Galli

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Photocatalysis

Sponsored by CATL, Cosponsored by COMP

In situ Characterization Tools

Sponsored by CATL, Cosponsored by COMP

Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

Sponsored by CINF, Cosponsored by COMP

WEDNESDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

R. E. Amaro, *Presiding*

1:30 COMP **471.** PROGNOSTIX: A pipeline for personalized diagnostics and drug. **J. Skolnick**

2:00 COMP **472.** Investigating allosteric regulation and cryptic pocket formation through enhanced sampling simulations. **F. Gervasio**

2:30 COMP **473.** Prediction on allosteric and cryptic sites on ligand-free protein structures. **S. Vajda**, D. Kozakov, D.R. Hall

3:00 Intermission.

3:20 COMP **474.** Computational riboswitch detection and design using inverse RNA folding simulations with ligand binding information. M. Drory, I. Kifer, S. Sengupta, Z. Yakhini, **D. Barash**

3:50 COMP **475.** Fine-tuned allosteric regulation of neuronal NMDA receptors with potential therapeutic importance. **N. Stanley**, A. Sinitskiy, B.D. Sellers, V.S. Pande

Section B

InterContinental San Francisco

Fremont

Material Science

Electron Transfer & Nanoparticles

C. M. Aikens, *Organizer*

M. Provorse, *Presiding*

1:30 COMP **476.** Functional mode hot electron transfer theory. J. Elenewski, J. Cai, W. Jiang, **H. Chen**

2:00 COMP **477.** Scaling relationships for nonadiabatic energy relaxation times in warm dense matter: Toward understanding the equation of state. **A.V. Akimov**

2:30 COMP **478.** Investigation of many-body correlation in excitonic and biexcitonic systems using electron-hole multicomponent coupled-cluster theory (eh-mcCC). B.H. Ellis, **A. Chakraborty**

3:00 COMP **479.** Unraveling excitation energy transfer mechanisms in plasmonic nanoantennas. **N. Ilawe**, M.B. Oviedo, B.M. Wong

3:30 Intermission.

4:00 COMP **480.** Luminescence properties of $Au_{38}(SH)_{24}$ and $Au_{22}SH_{18}$ nanoparticles. **K. Weerawardene**, C.M. Aikens

4:30 COMP **481.** Theoretical study of the chiroptical activity of BINAP– and DIOP– stabilized undecagold clusters. **N. Karimova**, C.M. Aikens

5:00 COMP **482.** Double ring tubular structures of boron clusters stabilized by metal atom doping: M@B_{14} (M = Cr, Fe, and Ni). **P. Saha**, A. Rahane, N. Sukumar, V. Kumar

‡*Cooperative Cosponsorship*

Section C

InterContinental San Francisco
Howard

Molecular Mechanics

Membrane-Interacting Proteins & Peptides

M. Feig, *Organizer*

S. Lindert, *Presiding*

1:30 COMP **483.** Structure-kinetic relationships of passive membrane permeation from multiscale modeling. **C. Dickson**, V. Hornak, R.A. Pearlstein, J. Duca

2:00 COMP **484.** Modeling permeability through outer-membrane channels in gram-negative pathogens. **S. Acosta-Gutierrez**, I. Bodrenko, S. Susruta, G. Malloci, M. Scorciapino, M. Ceccarelli

2:25 COMP **485.** Studying the substrate specificity and reactivity of MycG: A multifunctional enzyme. **S. Yang**, J.M. Grandner, M. Demars, D.H. Sherman, K.N. Houk

2:50 Intermission.

3:05 COMP **486.** Graded activation and free energy landscapes of a muscarinic G protein-coupled receptor. **Y. Miao**, J. McCammon

3:35 COMP **487.** Structural insights into conformation and dynamics of the cannabinoid CB2 receptor through an extended MD simulation of CP 55, 940–CB2 complex. **P. Pandey**, K. Roy, R.J. Doerksen

4:05 COMP **488.** Cell-scale computational modeling methodologies for living membranes. **J.V. Vermaas**, E. Tajkhorshid

4:35 COMP **489.** Oncogenic mutations differentially affect bax monomer, dimer, and oligomeric pore formation in the membrane. **M. Zhang**, J. Zheng, R. Nussinov, B. Ma

Section D

InterContinental San Francisco
Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

J. Larkin, *Presiding*

1:30 COMP **490.** QM cluster model examination of constrained biphenyl dihedral rotation within a modified threonyl-tRNA synthetase: A transition state trapped? T.J. Summers, **N.J. Deyonker**

2:05 COMP **491.** High-level characterization of the properties of R-X...π interactions in protein-ligand complexes. **K. Riley**, K. Tran

2:30 COMP **492.** Improved energy decomposition analysis for studying covalent bonds. **D.S. Levine**, M.P. Head-Gordon

2:55 Intermission.

3:10 COMP **493.** Developments in stochastic coupled cluster theory. **A.J. Thom**

3:35 COMP **494.** Electron propagator theory and correlation-bound anions. **J.V. Ortiz**

4:00 COMP **495.** Improving efficiency of semi-direct MP2 through oversubscription. **E. Fought**, V. Sundriyal, M. Sosonkina, T.L. Windus

4:25 COMP **496.** Development of a many-body carbon dioxide potential and its application to clusters up to $(CO_2)_{13}$. **O. Sode**

Section E

InterContinental San Francisco
Laurel Hill

Drug Design

Structure-Activity Relationships & Pharmacophores

M. R. Landon, Y. Tseng, *Organizers*

J. M. Spiriti, *Presiding*

1:30 COMP **497.** Combining protein interaction potentials with water analysis in structure-based design. **T. Cheeseright**, M.D. Mackey, G. Tedesco, S. Tomasio, P. Tosco

1:50 COMP **498.** Optimization of shape fingerprints for protein-ligand systems. **J. Zarnecka**, A.G. Leach, S.J. Enoch

2:10 COMP **499.** Deep learning profile-QSAR 2.0 IC_{50} predictions as accurate as 4-pt IC50s: Applications to polypharmacology. **E.J. Martin**, V. Polyakov, L. Tian

2:30 COMP **500.** Towards in-silica screening of molecule permeation through outer membrane channels in Gram-negative bacteria. I. Bodrenko, S. Acosta Gutierrez, T. D'Agostino, S. Samanta, S. Salis, G. Malloci, M. Scorciapino, **M. Ceccarelli**

2:50 Intermission.

3:10 COMP **501.** Withdrawn.

3:30 COMP **502.** GPCR activation: Principle component analysis as a diagnostic signature correlated with SAR. **D.L. Harris**, J.B. Thomas, Y. Zhang, E. Gay, S. Runyon

3:50 COMP **503.** Molecular simulation of EFdA and related analogs to determine the structural basis of HIV-1 drug resistance. **D. Das**, Y. Takamatsu, S. Kohgo, S. Hattori, H. Hayashi, K. Matsuda, S. Sarafianos, H. Mitsuya, K. Maeda

4:10 COMP **504.** Automated extraction of pharmacophores and toxophores from large-scale *in vitro* pharmacology data. **A. Dossetter**, E.J. Griffen, A.G. Leach, J. Stacey, L. Reid, S. Montague

Section F

InterContinental San Francisco
Nob Hill

State-of-the-Art Methods for Modeling Materials Chemistry

Cosponsored by CATL and MPPG‡

B. G. Janesko, J. A. Keith, *Organizers*, *Presiding*

1:30 COMP **505.** Towards a chemically accurate description of reactions of molecules with transition metal surfaces. **G. Kroes**

1:55 COMP **506.** Towards accurate and reliable simulations water at interfaces, and more…. **A. Michaelides**

2:20 COMP **507.** Understanding and eliminating delocalization error in transition metal chemistry. T.Z. Gani, Q. Zhao, **H.J. Kulik**

2:45 COMP **508.** Development of a general framework for coupling machine learning and *ab initio* approaches in materials chemistry. **A. Kolpak**

3:10 Intermission.

3:30 COMP **509.** ANAKIN-ME: A general purpose and chemically accurate deep learned potential. J.S. Smith, O. Isayev, **A.E. Roitberg**

3:55 COMP **510.** Efficient parallelization of the calculation of exact exchange for plane-wave DFT. **T.A. Barnes**, J. Deslippe, P. Kent, D. Prendergast

4:10 COMP **511.** Application of ab initio many-body perturbation theory with Gaussian basis sets to the singlet and triplet excitations of organic molecules. **S. Hamed**, T. Rangel, F. Bruneval, J. Neaton

4:25 COMP **512.** QM/MM simulations of TADF materials. **P. de Silva**, T. Zhu, T.A. Van Voorhis

4:50 COMP **513.** Accurate level alignment at molecule-metal interfaces from an optimally-tuned range-separated hybrid functional. **Z. Liu**, D.A. Egger, S. Refaely-Abramson, L. Kronik, J. Neaton

5:05 COMP **514.** Hybrid functional pseudopotentials. **L. Tan**, J. Yang, A.M. Rappe

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Transition Metal & Metal Oxide Catalysis

Sponsored by CATL, Cosponsored by COMP

Public-Private Partnerships: Fostering Drug Discovery & Data Sharing

Sponsored by CINF, Cosponsored by COMP

THURSDAY MORNING

Section A

InterContinental San Francisco
Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

M. P. Jacobson, *Presiding*

8:30 COMP **515.** Computer-aided discovery of allosteric modulators for a muscarinic G-protein-coupled receptor. **Y. Miao**, J. McCammon

9:00 COMP **516.** Structure-based design of allosteric K-Ras inhibitors. **A. Gorfe**

9:30 COMP **517.** Kinase allostery atlas. **D. Kozakov**

10:00 Intermission.

10:20 COMP **518.** Mechanisms for allosteric inhibition of protein tyrosine phosphatase 1B. **H.P. Hendrickson**, J. Lipchock, B. Douglas, I. Rivalta, N. Ten, V.S. Batista, J. Loria

10:50 COMP **519.** Order in the disordered polybasic domain of K-Ras. **P.S. Srivastava**, Y. Zhou, H. Liang, K. Cho, J. Hancock, A. Gorfe

11:20 COMP **520.** Exploring the therapeutic landscape of chromatin via integrative computational modeling: An allosteric regulation from transition metal agents. **G. Palermo**, Z. Adhireksan, T. Riedel, Z. Ma, R. Muhammad, U. Roethlisberger, P. Dyson, C. Davey

Section B

InterContinental San Francisco
Fremont

Material Science

Functional Materials & High-Throughput Screening Methods

C. M. Aikens, *Organizer*

N. Saikia, *Presiding*

8:30 COMP **521.** Assessing the potential of $LaCrO_3$ as a *p*-type semiconducting oxide. **A.L. Gavin**, G.W. Watson

9:00 COMP **522.** Interatomic potential for a perovskite electrolyte derived from first principles. **A.K. Lucid**, G.W. Watson

9:30 COMP **523.** High-throughput screening of transparent conducting oxides. **C. Sutton**, R.J. Baldock, L.M. Ghiringhelli, M. Scheffler

10:00 COMP **524.** Gibbs energies of solids through materials informatics. **C. Bartel**, A. Deml, S. Miller, J. Rumptz, A.W. Weimer, S. Lany, C. Musgrave, V. Stevanovic, A. Holder

10:30 Intermission.

11:00 COMP **525.** *In silico* design of 3D covalent organic frameworks for gas adsorption applications. **R. Mercado**, R. Fu, B. Smit

11:30 COMP **526.** Understanding of spectacular gas adsorption/separation phenomena in metal-organic frameworks. R. Pillai, **G. Maurin**, S. Krause, S. Kaskel, J. Yoon, J. Chang

12:00 COMP **527.** Cryptands as cathode materials for batteries. **H. Gokturk**

Section C

InterContinental San Francisco
Howard

Molecular Mechanics

Force Fields

M. Feig, *Organizer*

F. Tofoleanu, *Presiding*

8:30 COMP **528.** Toward more accurate force fields through direct chemical perception. **D.L. Mobley**, C. Bannan, C. Zanette, C.I. Bayly, J.D. Chodera, M.R. Shirts, J. Fass, B. Manubay, P. Eastman, M.K. Gilson

9:00 COMP **529.** Systematic exploration of hydration thermodynamics and kinetics of various approximate polarization schemes. **F.C. Pickard**, A.C. Simmonett, G. Koenig, J. Huang, B. Brooks, J.W. Ponder

9:30 COMP **530.** Consistent integration of experimental and ab initio data into effective molecular force fields. **L. Vlcek**

10:00 Intermission.

10:15 COMP **531.** Refined AMBER force field (FUJI) force field for phospholipids. N. Kamiya, **H. Fujitani**

10:45 COMP **532.** Force field development for water interacting with Pt surfaces. **A.W. Goetz**, R.F. de Morais, B. Schweitzer, P. Fleurat-Lessard, P. Sautet, S. Steinmann, C. Michel

11:15 COMP **533.** Biocompatible force field for thiolated gold nanoclusters in macromolecular environments. **J. Gascon**

11:45 COMP **534.** Thermodynamic calculations of cyclodextrin host-guest binding: A comprehensive evaluation of force field performance. **N.M. Henriksen**, M.K. Gilson

Section D

InterContinental San Francisco

Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer*

J. J. Foley, *Presiding*

8:30 COMP **535.** Strong-field ionization in molecules using range-separated time-dependent density functional theory. A. Sissay, A. Bruner, P. Abanador, F. Mauger, M. Gaarde, K. Schafer, **K. Lopata**

9:05 COMP **536.** Non-linear conductivity of metals from real-time time-dependent density functional theory. **X. Andrade**, A.A. Correa

9:30 COMP **537.** Excited state absorption from real-time time-dependent density functional theory simulations: Predicting molecular optical response by excited state density propagation. **D.N. Bowman**, J. Asher, S. Fischer, N. Govind, C.J. Cramer

9:55 COMP **538.** Quantum mechanical models with statistical effects and statistical models without quantum effects. **J. Parkhill**

10:30 Intermission.

10:45 COMP **539.** Linear-response, stability and single-particle excited states in noncollinear spin density functional theory. **G. Scalmani**, F. Egidi, M.J. Frisch, X. Li

11:10 COMP **540.** Many-pair expansion: A systematically improvable correction scheme for including strong and long-range correlations in DFT. **P. de Silva**, T. Zhu, T.A. Van Voorhis

11:35 COMP **541.** Unconventional Kohn-Sham theory: Implementation and application of complex-restricted and general orbital density functional theories. **L.W. Bertels**, M.P. Head-Gordon

12:00 COMP **542.** Polarizabilities of π-conjugated chains revisited: Improved results from broken-symmetry, range-separated DFT. **B.M. Wong**, M.B. Oviedo, N. Ilawe

Section E

InterContinental San Francisco

Laurel Hill

Drug Design

Applications

M. R. Landon, Y. Tseng, *Organizers*

M. Korczynska, *Presiding*

8:30 COMP **543.** Molecular simulations disclose a novel mode of one-stranded intercalation in nucleosomes that is DNA topology dependent. **G. Palermo**, Z. Ma, Z. Adhireksan, B. Murray, T. von Erlach, P. Dyson, C. Davey, U. Roethlisberger

8:50 COMP **544.** Withdrawn.

9:10 COMP **545.** Rational bioavailability design: Optimizing bioavailability in lead op with Global Sensitivity Analysis of Physiologically-Based PK (GSA of PBPK). **E.J. Martin**, P. Daga, B. Madej

9:30 COMP **546.** Is alternative binding sapping the strength of current oxime countermeasures? **B.J. Bennion**, T. Carpenter, F.C. Lightstone, T. Nguyen, C.A. Valdez

9:50 Intermission.

10:10 COMP **547.** Rational bioavailability optimization using physiologically-based pharmacokinetics simulations. **B.D. Madej**, E.J. Martin

10:30 COMP **548.** Ligand based drug discovery of novel dengue-2 NS2B-NS3 protease inhibitors. M.M. Nawi, S. Abdul Hamid, M. Hariono, R. Othman, S. Othman, R. Yusuf, N.A. Rahman, **H. Wahab**

10:50 COMP **549.** Virtual fragment screening and linking discovers Jumonji histone demethylase inhibitors. **M. Korczynska**, D.D. Le, M. Siklos, N. Younger, E. Gregori-Puigjané, A. Tumber, T. Krojer, S. Velupillai, C. Gileadi, R. Nowak, E. Iwasa, S.B. Pollock, I. Ortiz Torres, U. Oppermann, B. Shoichet, D.G. Fujimori

11:10 COMP **550.** Molecular drug design targeting a bacterial RNA structure: Atomic resolution mechanistic studies of highly selective unnatural ligand mimic of the *E. coli* FMN riboswitch. **L. Xiao**

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Biomass Catalysis

Sponsored by CATL, Cosponsored by COMP

THURSDAY AFTERNOON

Section A

InterContinental San Francisco

Twin Peaks

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Mechanisms & Molecular Simulations

Cosponsored by PHYS

C. Chang, G. Verkhivker, *Organizers*

S. Vajda, *Presiding*

1:30 COMP **551.** Glutamate receptor ion channel activation mechanism revealed by computer experiment. **X. Wu**, B. Brooks

2:00 COMP **552.** CaMKII: A molecular dynamics study of the effects of phosphorylation on its dodecameric form. **I. General**

2:30 COMP **553.** Computational tools for the evaluation of laboratory-engineered biocatalysts. **M. Garcia-Borras**, A. Romero-Rivera, S. Osuna

3:00 Intermission.

3:20 COMP **554.** Constant-pH simulations on capability class computers: First applications. **B. Radak**, J. Phillips, W. Jiang, K. Schulten, B. Roux

3:50 COMP **555.** Directional motion in chiral molecules out of equilibrium. **D. Slochower**, M.K. Gilson

Section B

InterContinental San Francisco

Fremont

Material Science

Surfaces & Catalysts

C. M. Aikens, *Organizer*

A. Shamloo, *Presiding*

1:30 COMP **556.** Growth mechanism of small PdGa bimetallic clusters on MgO (100) surface. **N. Kumar**, D. Chattaraj, I. Kaul, C. Majumder, P. Ghosh

2:00 COMP **557.** Surface characterization of supported catalysts: The interplay between modeling and experiments. **V. D'Anna**, C. Michel, P. Sautet

2:30 COMP **558.** Density-functional study of the $La_2Zr_2O_7$ low-index faces. **Y. Mantz**, Y. Duan

3:00 COMP **559.** Formation and diffusion of oxygen vacancies in complex transition-metal oxides from diffusion quantum Monte Carlo. **J.A. Santana**, J. Krogel, P. Kent, F. Reboredo

3:30 Intermission.

4:00 COMP **560.** Decorating the (110) facet of rutile-type crytallites with CH_4: A first-principles investigation. **A. Abbaspour Tamijani**

4:30 COMP **561.** Dynamics of self-assembled guanine nucleobases on graphene. **N. Saikia**, K. Waters, S.P. Karna, R. Pandey

5:00 COMP **562.** Computational study of the binding of methane and aromatic amino acids with graphene. **T. Dinadayalane**, J. Lazare, D. Daggag

Section C

InterContinental San Francisco

Howard

Molecular Mechanics

Protons & Electrons

M. Feig, *Organizer*

A. Levit, *Presiding*

1:30 COMP **563.** Assessing and optimizing efficiency in nonequilibrium molecular dynamics/Monte Carlo simulations. **B. Radak**, B. Roux

1:55 COMP **564.** High-performance molecular dynamics at constant pH and constant redox potential using AMBER. **V.D. Cruzeiro**, M. Amaral, A.E. Roitberg

2:20 COMP **565.** Unraveling the dynamics of the redox conformational protection of nitrogenase. **F. Feixas**, M. Gimferrer, P. Salvador, M. Garcia-Borras

2:45 COMP **566.** Self-activated mechanism for efficient nucleic acids polymerization. V. Genna, P. Visossich, E. Ippolito, P. Carloni, **M. Devivo**

3:10 Intermission.

3:25 COMP **567.** NH_3 binding to the S_2 state of the O_2-evolving complex of Photosystem II points at H_2O binding during the $S_2 \rightarrow S_3$ transition: Insights from QM/MM, EXAFS, and femtosecond x-ray diffraction. **M. Askerka**, D. Vinyard, J. Wang, G.W. Brudvig, V.S. Batista

3:50 COMP **568.** Thermal isomerization relaxation of azobenzene derivatives studied with QM/MM and transition path sampling. **A. Muzdalo**, P. Saalfrank, **M. Santer**

4:15 COMP **569.** Structural and electronic features of Mg^{2+}-RNA binding motifs: Insights from combined classical molecular dynamics and quantum mechanics simulations. **L. Casalino**, G. Palermo, N. Abdurakhmonova, U. Roethlisberger, A. Magistrato

Section D

InterContinental San Francisco

Cathedral Hill

Quantum Mechanics

A. E. DePrince, *Organizer, Presiding*

1:30 COMP **570.** Large-scale selected configuration interaction based on a Davidson-Liu flow. **R.M. Parrish**, T.J. Martinez

2:05 COMP **571.** Complex basis functions for metastable electronic states: Methodology and applications. **A. White**, C.W. McCurdy, M.P. Head-Gordon

2:30 COMP **572.** Excited states for orbital-optimized second-order perturbation theory. **E. Ramos**, M.P. Head-Gordon

2:55 COMP **573.** Unique electronic dynamics from scattering mediated absorption. **J.J. Foley**

3:30 Intermission.

3:45 COMP **574.** Geminals for dispersion interactions and long-range correlation. **J.F. Gonthier**, M.P. Head-Gordon

4:10 COMP **575.** Hybrid classical/quantum approach for large-scale studies of quantum systems with density matrix embedding theory. **N.C. Rubin**

4:35 COMP **576.** Examining the excited state deactivation pathways of 5-hydroxymethylcytosine. **J. Mato**, K. Keipert, M.S. Gordon

5:00 COMP **577.** Theoretical studies of the catalytic transition metal nanoparticles with flexible structures. **G. Wei**, Z. Liu

Section E

InterContinental San Francisco

Laurel Hill

Drug Design

Applications

M. R. Landon, Y. Tseng, *Organizers*

P. Bisignano, *Presiding*

1:30 COMP **578.** Exploiting water density fluctuations in ion channel drug design. **E. Gianti**, L. Delemotte, M.L. Klein, V. Carnevale

1:55 COMP **579.** Adding pharmacophores to shape and electrostatics - too much of a good thing? **T. Cheeseright**, M.D. Mackey, S. Tomasio

2:20 COMP **580.** Investigation of the molecular electrostatic potentials and the average electron densities of non-classical bioisosteres. **A.A. Arabi**, C.F. Matta

2:45 Intermission.

3:05 COMP **581.** From protons to fragments with XModeScore: How we can use x-ray data coupled with quantum mechanics to explore these elusive species in binding. **L. Westerhoff**, O. Borbulevych

3:30 COMP **582.** Key role of the β5-β6 loop conformation in the substrate specificity of OXA-48–like enzymes: Implications for the β-lactamase-mediated antibiotic resistance. L. Dabos, R. Bonnin, L. Dortet, T. Naas, **B.I. Iorga**

3:55 COMP **583.** *In silico* analysis of Z-77 variants for optimal inhibition of *E. coli* beta-glucuronidase. **K.T. Lane**, H. Gullickson

‡ *Cooperative Cosponsorship*

4:20 COMP **584.** 2A but not 2B: Towards structure-based discovery of new Serotonin receptor modulators. **A. Levit**, D. Wacker, J.D. McCorvy, B.L. Roth, B. Shoichet

Designed Catalysis: Materials Genome Approach to Heterogeneous Processes

Machine Learning Tools for Catalyst Genome

Sponsored by CATL, Cosponsored by COMP

ENFL

Division of Energy and Fuels

D. J. Heldebrant, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials (see *CATL,* Mon, Tue)

Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy (see *CELL*, Mon)

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis (see *CATL,* Mon, Tue, Wed)

Rising Star Award Symposium (see *WCC, Mon*)

Science for a Sustainable Energy Future: Energy Storage (see *PRES,* Mon)

SOCIAL EVENTS:

Executive Committee Meeting, 4:00 PM: Sun

Dinner, 6:00 PM: Tue

BUSINESS MEETINGS:

Program Meeting, 12:00 PM: Sun

Business Meeting & Social, 12:00 PM: Mon

SUNDAY MORNING

Section A

Grand Hyatt San Francisco

Belvedere

Advanced Analytical Techniques for Determination of Minor & Trace Elements in Petroleum Value Chain

J. Casey, *Organizer*

J. Nelson, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **1.** Recent improvements of the ICP/MS capabilities of the 8800 for the petroleum industry. **L. Charles-Philippe**, C. Sanchez Rodriguez, F. Chainet, M. Milliland, L. Ayouni, S. Carbonneaux, J. Todoli, A. Desprez

9:20 ENFL **2.** Determination of trace elements in petroleum feedstocks by ICP-MS: From total content towards their distribution. **F.A. Lopez-Linares**, **L. Poirier**, M.M. Boduszynski, C.E. Rechsteiner, M. Moir, D. Leong, C.F. Ovalles, E. Rogel, J. Nelson

9:50 ENFL **3.** Use of GC-ICP-MS for analysis of petroleum and petrochemicals in a service laboratory. **W. Geiger**, B. McElmurry, J. Anguiano

10:20 Intermission.

10:40 ENFL **4.** Using the MS/MS capabilities of the Agilent 8900 ICP-QQQ for ultra-trace analysis of elements in the petroleum value chain. **M. Kelinske**, J. Nelson

50 high to low-abundance minor, trace and ultra-trace elements in crude oils by ICP-OES and QQQ-ICP-MS: New methods of geochemical fingerprinting. **J. Casey**, Y. Gao

11:30 ENFL **6.** Simultaneous measurement of twenty-five trace elements in aviation turbine engine and diesel fuels by inductively coupled plasma tandem mass spectrometry. **G.T. Eldridge**, R.K. Larsen, M.E. Peretich, R.P. Shah, A. Metz

11:55 ENFL **7.** Measurement of copper in aviation turbine engine fuel by inductively coupled plasma tandem mass spectrometry and comparison to graphite furnace atomic absorption spectrometry. **A. Metz**, R.K. Larsen, M.E. Peretich, G.T. Eldridge

Section B

Grand Hyatt San Francisco

Filmore C

C1 Catalysis

Cosponsored by CATL

K. Ding, N. Kumar, *Organizers*

J. J. Spivey, *Organizer, Presiding*

K. Ding, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **8.** Strategies to selectively oxidize methane to methanol. **J.A. Lercher**

9:15 ENFL **9.** Nature of active sites and mechanism of selective methane oxidation by Cu and Fe-modified zeolite catalysts. A. Szecsenyi, G. Li, J. Gascon, E. Hensen, **E. Pidko**

9:35 ENFL **10.** Copper oxide clusters as active catalytic sites of CuMOR zeolite for methane to methanol conversion: Size matters? **D. Palagin**, A.J. Knorpp, A.B. Pinar, M. Ranocchiari, J.A. van Bokhoven

9:55 ENFL **11.** Defining the active sites of low-temperature methane hydroxylation in iron and copper zeolites. **B.E. Snyder**, P. Vanelderen, J. Woertink, B.F. Sels, R.A. Schoonheydt, E.I. Solomon

10:15 Intermission.

10:30 ENFL **12.** Biological methane oxidation. **A.C. Rosenzweig**

11:10 ENFL **13.** Chemical transformation of shale gas components under mild conditions in liquid. **F. Tao**

11:40 ENFL **14.** Direct conversion of methane to methanol and ethanol. C. Okolie, Y. Belhseine, L. Kovarik, E. Stavitski, **C. Sievers**

Section C

Grand Hyatt San Francisco

Orpheum

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Cosponsored by CATL, MPPG‡ and PMSE

Y. H. Hu, R. T. Koodali, H. Wang, *Organizers*

Y. Li, Y. Ng, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **15.** Acid treatment enables suppression of electron-hole recombination in hematite for photoelectrochemical water splitting. **Y. Li**

9:15 ENFL **16.** Nanostructured hybrid electrodes for photoelectrochemical CO_2 conversion: Synthetic aspects and structure-property relationships. E. Kecsenovity, A. Kormanyos, B. Endrodi, **C. Janaky**

9:45 ENFL **17.** Vitamin C as a surface modifier for solar hydrogen production. **T. Dramstad**, D. Harts, B. Selvaratnam, R.T. Koodali

10:05 Intermission.

10:15 ENFL **18.** Bismuth-based ternary oxide for photocatalytic and photoelectrochemical water splitting. **Y. Ng**

10:55 ENFL **19.** Engineering nanomaterials for energy conversion. **X. Zheng**

11:25 ENFL **20.** Structure and properties of hydrothermally prepared MoS_2 thin films on gold substrate. **A.S. Ichimura**, R. Sfadia, J. Macias, B. Gunn, A. Newaz, C. Tassone

11:55 ENFL **21.** Photoelectrocatalytic reduction of CO_2 on organic/inorganic nanocomposite photoelectrodes. **A. Kormanyos**, D. Hursan, K. Rajeshwar, C. Janaky

12:15 Concluding Remarks.

Section D

Grand Hyatt San Francisco

Curran

Catalysis for Unconventional Energy Sources

Cosponsored by CATL and MPPG‡

X. Wang, *Organizer*

Y. H. Hu, *Organizer, Presiding*

F. Li, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **22.** Thermochemical studies of catalyst stability and function. **A. Navrotsky**

9:15 ENFL **23.** Mn-containing mixed metal oxides for chemical looping oxidative dehydrogenation of ethane. **F. Li**

9:45 ENFL **24.** Sustainable production of bio-based alcohols, esters, aromatics and polyols from lignin: The art of the right catalyst. **Y. Li**, R. Ma, X. Ma

10:15 Intermission.

10:30 ENFL **25.** Visible light photocatalytic production of H_2. **Y.H. Hu**

11:10 ENFL **26.** Catalyzing energy storage for optimum use of intermittent renewable energy resources. **M. Isaacson**

11:50 ENFL **27.** Light absorbers, interfaces, and catalysts for solar-to-fuel conversion: First-principles calculations. **Y. Ping**

12:20 Concluding Remarks.

Section E

Grand Hyatt San Francisco

Sequoia

Subsurface Technologies for Recovery of Fossil & Geothermal Energy

Cosponsored by CATL and GEOC

C. Fernandez, M. A. Reynolds, *Organizers*

C. Fernandez, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **28.** Results from Newberry volcano EGS demonstration, 2010-2015. **T. Cladouhos**, S. Petty, M.W. Swyer, M. Uddenberg, K. Grasso, Y. Nordin

9:10 ENFL **29.** TOGA: Compositional simulation of three-phase, multi-component, and non-isothermal processes for carbon dioxide utilization and storage in partially depleted oil and gas reservoirs. **C. Oldenburg**, L. Pan

9:35 ENFL **30.** Experiments, simulations, and reduced physics modeling for risk assessment of well integrity at CO_2 storage sites. **N. Huerta**, J. Iyer, V. Vasylkivska, S.A. Carroll, W.L. Du Frane, B. Kutchko, L. Li, H. Mason, P. Roy, S.D. Walsh

10:00 ENFL **31.** Development of an electrochemical sensor for downhole tracer and pH measurements in real-time. **R.F. Hess**, B. Klamm, L. Goldfarb, W.C. Corbin, T.J. Boyle, W.G. Yelton, A.T. Cashion

10:25 Intermission.

10:30 ENFL **32.** Caustic-cracking likely cause of failure in geothermal production casing – well redesign and cementing changes key to replacement well success. **D. Bour**, M. Gao, R. Krishnamurthy, R. Rudolf, R. Hausler

11:05 ENFL **33.** Made-to-order metal-organic frameworks for gas capture and storage. **M. Eddaoudi**, D. Alezi, Y. Belmabkhout

11:30 ENFL **34.** Self-healing polymer-cement composites for geothermal wells and their properties. **M. Childers**, K.A. Rod, M.T. Nguyen, M. Elbakhshwan, S. Gill, W. Um, J. Chun, V. Glezakou, T.J. Roosendaal, T. Wietsma, P.K. Koech, N. Huerta, B. Kutchko, C. Fernandez

11:55 ENFL **35.** Microbial consortia encapsulated with ultralight kaolinite proppant for in-situ microbially enhanced methane recovery. **K. Han**, J. Fuertez, A. Szendrei, V. Nguyen, J. McLennan, T.D. Sparks

12:20 Concluding Remarks.

Section F

Grand Hyatt San Francisco

Cypress

Computations for CO2 Capture, Conversion & Sequestration

Cosponsored by CATL, COMP, GEOC and MPPG‡

V. Glezakou, R. Rousseau, *Organizers*

S. Raugei, *Presiding*

8:30 ENFL **36.** Reaction dynamics of CO_2 in amine solutions from DFT-based simulations. **W. Andreoni**, C. Ma, F. Pietrucci

9:15 ENFL **37.** Understanding the structure and dynamics of CO2-reactive aprotic heterocyclic anion ionic liquids: A molecular simulation study. E. Maginn, **Q. Sheridan**, W.F. Schneider

10:00 Intermission.

10:30 ENFL **38.** March toward task-specific CO_2 capture solvents. **V. Glezakou**, R. Rousseau, D.C. Cantu, D. Malhotra, D.J. Heldebrant, P.K. Koech

11:05 ENFL **39.** Polymorphic transitions of CO_2 molecular crystals: Thermodynamics, kinetics and confinement effects. I. Gimondi, **M. Salvalaglio**

Cellulose Structure & Biosynthesis In the Plant Cell Wall

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Electrocatalysis for Energy Generation & Storage

Oxygen Reduction

Sponsored by CATL, Cosponsored by ENFL

SUNDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Belvedere

Advanced Analytical Techniques for Determination of Minor & Trace Elements in Petroleum Value Chain

J. Casey, *Organizer*

J. Nelson, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **40.** Comparison of existing methods for analysis of finished biofuels using Microwave Plasma Atomic Emission Spectroscopy (MP-AES) - moving the biofuels industry forward. **T. Alleman**, G. Gilleland

2:00 ENFL **41.** Multi-elemental determination of petroleum products using the Agilent 5110 ICP-OES. **E. Kulikov**, N. Drvodelic, P. Lowenstern

2:25 ENFL **42.** Elemental analysis of asphaltenes by tandem LIBS- LA-ICP-OES. F.A. Lopez-Linares, **J. Gonzalez**, J.R. Chirinos, D. Oropeza, D. Quarles, C. Ovalles, E. Rogel, R.E. Russo

2:50 ENFL **43.** Determination of total chloride in petroleum crude samples by Combustion Ion Chromatography (CIC). M. Dutta, **A. Pathiparampil**, S.H. Roby, F.A. Lopez-Linares

Section B

Grand Hyatt San Francisco
Filmore C

C1 Catalysis

Cosponsored by CATL

K. Ding, J. J. Spivey, *Organizers*

N. Kumar, *Organizer, Presiding*

K. Ding, *Presiding*

1:30 ENFL **44.** Methane activation by oxide catalysts: The role of coadsorption. **H. Metiu**, S. Chretien, H.H. Kristoffersen

2:10 ENFL **45.** *In-situ* studies of Ni-Ce-O catalysts for the reforming of methane: Insights from TR-XRD, XANES, and NAP-XPS. **J. Rodriguez**, Z. Liu, S.D. Senanayake, D. Grinter

2:50 ENFL **46.** Au@PdO_x with PdO_x-rich shell and Au-rich core embedded in Co_3O_4 nanorods for catalytic oxidation of methane. **Y. Zhu**

3:10 Intermission.

3:25 ENFL **47.** Oxidative coupling of methane on Na_2WO_4/Mn/SiO_2 catalyst: Mechanistic studies and a new reactor concept. **R. Schomaecker**

4:05 ENFL **48.** Theoretical study on oxidative coupling of methane using MgO. **H. Aljama**, J.K. Norskov, F. Abild-Pedersen

4:25 ENFL **49.** Oxidative coupling of methane over tungsten-based nanomaterials. **W. Liu**, W. Ralston, G. Melaet, G.A. Somorjai

4:45 ENFL **50.** Pulsed regeneration of Mo/HZSM-5 methane dehydroaromatization catalysts. **E. Hensen**, N. Kosinov

Section C

Grand Hyatt San Francisco
Orpheum

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Cosponsored by CATL, MPPG‡ and PMSE

Y. H. Hu, R. T. Koodali, H. Wang, *Organizers*

Y. Ng, N. Wu, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **51.** Tuning charge separation and migration in semiconductors for solar energy conversion. **N. Wu**

2:15 ENFL **52.** Nanostructured carbon based materials for photocatalytically reduce carbon dioxide to fuels. **H. Li**

2:35 ENFL **53.** Withdrawn.

2:55 ENFL **54.** Finite temperature modeling of metal oxides for solar thermochemical water splitting. **S. Miller**, K. Sun, A.W. Weimer, C. Musgrave

3:15 Intermission.

3:25 ENFL **55.** Multicomponent transport in membranes for solar fuels devices. **D. Miller**, B. Beckingham

3:45 ENFL **56.** Phase-pure and photoactive scheelite from atomic layer deposition. **M. Stefik**

4:05 ENFL **57.** Reinforced perovskite solar cells designed with integrated polymer scaffolding for robust, efficient photovoltaics. **A. Printz**, N. Rolston, B. Watson, R. Dauskardt

4:25 ENFL **58.** Empirical extraction of the spatial collection efficiency of photovoltaic and photoelectrochemical devices. **G. Segev**, H. Dotan, D. Klotz, D. Grave, Y. Levy, B. Stannowski, A. Rothschild

4:45 ENFL **59.** Photothermal-enhanced catalysis in core-shell plasmonic hierarchical Cu_7S_4 microsphere@ zeolitic imidazole framework-8. **F. Wang**, Y. Huang, Q. Li, Y. Wang, D. Xu

5:05 ENFL **60.** Photoelectrochemical properties and behavior of α-$SnWO_4$ photoanodes synthesized by hydrothermal conversion of WO_3 films. **Z. Zhu**, P. Sarker, C. Zhao, L. Zhou, R. Grimm, M. Huda, P. Rao

5:25 Concluding Remarks.

Section D

Grand Hyatt San Francisco
Curran

Catalysis for Unconventional Energy Sources

Cosponsored by CATL and MPPG‡

Y. H. Hu, X. Wang, *Organizers*

M. Fan, X. Fan, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **61.** Catalyst design for liquid fuels from lignin: Hydrogenolysis without hydrogenation. **S.L. Scott**, Z.R. Jones, A. Chamas, L. Qi, M.B. Foston

2:15 ENFL **62.** Non-conventional: Catalytic upgrading of biomass pyrolysis vapour enabled by non-conventional energy (microwave). **X. Fan**

2:45 ENFL **63.** Strategies of removing surface states from photoanodes. Y. Li, X. Yun, H. Chen, **Y. Li**

3:15 ENFL **64.** High-yield synthesis of Pt-based two-dimensional nanoplates for methanol electro-oxidation reaction. **L. Chen**, Q. Zhang

3:35 Intermission.

3:50 ENFL **65.** New approach to reduction in CO_2 capture cost. **M. Fan**, M.A. Assiri, S. Toan, Q. Lai, A.G. Russell

4:30 ENFL **66.** Synthesis and characterization of high density multicyclic fuels based on sesquiterpanes and alkyl diamondoids. **B.G. Harvey**, K.W. Harrison, M.C. Davis, W.W. Merriman

5:00 Concluding Remarks.

Section E

Grand Hyatt San Francisco
Sequoia

Innovative Chemistry & Materials for Electrochemical Energy Storage

Cathode Materials

Cosponsored by MPPG‡ and PMSE

J. Guo, E. Pomerantseva, *Organizers*

Y. Mo, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **67.** Combining reversible oxygen charge transfer and Li-excess to achieve high capacity cathodes. **G. Ceder**

2:05 ENFL **68.** Conversion cathodes for next-generation Li and Li-ion batteries. E. Zhao, F. Wu, J. Lee, H. Kim, W. Gu, **G. Yushin**

2:35 ENFL **69.** Withdrawn.

2:55 ENFL **70.** Cu(bpy)V_4O_{10}: A 3D metal-organic framework as a cathode material for Li-ion batteries. **H. Zhou**, T. Young, S. Ang, T. Froedge, B. Yan

3:15 Intermission.

3:25 ENFL **71.** In situ TEM studies of electrochemistry at nanoscales. **R. Shahbazian Yassar**

3:55 ENFL **72.** Sodium-ion Batteries (SIB): Battery systems poised for grid storage. **C.S. Johnson**, E. Lee

4:25 ENFL **73.** Withdrawn.

4:55 ENFL **74.** Li-O_2 batteries based on oxyhalogen-sulfur chemistry. **X. Wang**, S. Meng

Section F

Grand Hyatt San Francisco
Cypress

Computations for CO2 Capture, Conversion & Sequestration

Cosponsored by CATL, COMP, GEOC and MPPG‡

V. Glezakou, R. Rousseau, *Organizers*

C. Skylaris, *Presiding*

1:30 ENFL **75.** Aminosilicone CO_2 capture solvents. **R.J. Perry**

2:15 ENFL **76.** Dual nature of extended solvent structure in CO_2-binding organic liquids: Thermodynamic vs kinetic stability. **D.J. Heldebrant**, D. Cantu, D. Malhotra, V. Glezakou, R. Rousseau, P.K. Koech

2:50 ENFL **77.** Energetically efficient non-aqueous amine-based solvents as carbon dioxide capture material. **D. Malhotra**, P.K. Koech, D.J. Heldebrant, V. Glezakou, D.C. Cantu, R. Rousseau, F. Zheng, M. Bearden

3:15 ENFL **78.** Computational aided design and synthesis of advanced carbon capture solvents. **J. Page**, D. Malhotra, D.C. Cantu, P.K. Koech, V. Glezakou, R. Rousseau, D.J. Heldebrant

3:40 Intermission.

4:00 ENFL **79.** CO_2 interactions for capture, conversion, or sequestration: From proteins and metal organic frameworks to scrubbers and beyond. **A.K. Wilson**

4:35 ENFL **80.** Weak interactions of CO_2 with functional groups of porous materials: Computational studies with correlated methods. **K.D. Vogiatzis**

5:05 ENFL **81.** New advances in carbon dioxide capture using diamine-appended metal-organic frameworks. **P.J. Milner**, J.R. Long

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Cellulose Structure & Biosynthesis

Evolution of Synthases & Fine Structure of Microfibrils

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Electrocatalysis for Energy Generation & Storage

CO_2 Reduction

Sponsored by CATL, Cosponsored by ENFL

MONDAY MORNING

Section A

Grand Hyatt San Francisco
Belvedere

Advances in Chemistry of Energy & Fuels

Separations

D. J. Heldebrant, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **82.** Controlling cooperative CO_2 adsorption in diamine-appended Mg_2(dobpdc) metal–organic frameworks. **R.L. Siegelman**, T. McDonald, M.I. Gonzalez, J. Martell, P.J. Milner, J.A. Mason, J.R. Long

8:55 ENFL **83.** Polyphosphazene based membranes for gas separations. **H.B. Nulwala**, Z. Li, D. Luebke, H. Allcock

9:15 ENFL **84.** Synthesis of a novel monolith combined activated carbon and zeolite-NaUSY for CO2 capture by Electric Swing Adsorption (ESA). **Q. Zhao**, F. Wu, P. Webley

9:35 ENFL **85.** DFT studies of CO_2 reduction pathways on Cu-based electrodes. **A.R. Asthagiri**

9:55 ENFL **86.** Fabrication of zeolite membranes for propylene/propane separation. **S. Shrestha**, P.K. Dutta

10:15 ENFL **87.** Catalytic removal of eibenzothiophene using $CoMoS_2$ synthesized using elemental sulfur. **J.G. Parsons**, J.S. Sollner, D.F. Gonzalez, J.H. Leal, T.M. Eubanks

10:35 ENFL **88.** Hydrate formation in microcapsules for temperature-sensitive release of encapsulants. **Y. Seo**, J. Park, S. Kim, S. Lee

‡ *Cooperative Cosponsorship*

10:55 ENFL **89.** Dynamic windows based on reversible metal electrodeposition with fast switching, neutral color, and excellent durability. **C. Barile**, T.S. Hernandez, M.T. Strand, D.J. Slotcavage, M.D. McGehee

11:15 Concluding Remarks.

Section B

Grand Hyatt San Francisco

Filmore C

C1 Catalysis

Cosponsored by CATL

K. Ding, J. J. Spivey, *Organizers*

N. Kumar, *Organizer, Presiding*

K. Ding, *Presiding*

8:30 ENFL **90.** Unexpected C1 catalysis. **P.C. Stair**

9:10 ENFL **91.** Understanding the role of interfaces in gold nanocluster catalysis through gas phase CO oxidation. **Z. Wu**

9:40 ENFL **92.** Synergy and anti-synergy between palladium and gold in nano-particles dispersed on a reducible support. **J. Carter**, S. Althahban, E. Nowicka, S. Freakley, D. Morgan, P. Shah, S. Golunski, C.J. Kiely, G. Hutchings

10:00 ENFL **93.** Role of water in CO oxidation and PROx over Au catalysts: Developments in hydrogen purification from methane. **B.D. Chandler**, J. Saavedra, T. Whittaker, C. Pursell

10:20 Intermission.

10:30 ENFL **94.** Methanol to gasoline transformation study over modified zeolite. **E. Sulman**, V. Doluda, N. Lakina, M. Sulman

10:50 ENFL **95.** Promotion mechanisms of iron oxide-based high temperature water–gas shift catalysts by chromium and copper. M. Zhu, T. Rocha, T. Lunkenbein, R. Schloegl, A. Knop-Gericke, **I.E. Wachs**

11:30 ENFL **96.** Conversion of methanol on zeolites containing transition metals. **E.P. Schreiner**, R.F. Lobo

11:50 ENFL **97.** Mechanistic understanding of H-MOR with enhanced stability for carbonylation of dimethyl ether. **Y. Li**, S. Huang, X. Ma

12:10 ENFL **98.** Impact of copper oxidation states on the reactivity in partial oxidation of methanol. **H. Chi**, C.M. Andolina, J. Li, G. Zhou, G. Veser, J. Yang

Section C

Grand Hyatt San Francisco

Orpheum

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Cosponsored by CATL, MPPG² and PMSE

R. T. Koodali, H. Wang, *Organizers*

Y. H. Hu, *Organizer, Presiding*

G. Cao, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **99.** Control and understand the impacts of nano and microstructures on perovskite solar cell performance. **G. Cao**

9:15 ENFL **100.** Aliphatically linked conjugated small molecules for crystal structure engineering and stability enhancement in organic solar cell. **X. Jeanbourquin**, A. Gasperini, A. Rahmanudin, K.A. Sivula

9:35 ENFL **101.** Assessing the use of polymer/ceramic composites as a hybrid material for supercapacitor separator. **E.O. Ortiz-Quiles**, C.O. Alvarez-Sanchez, J. Lasalde-Ramírez, R. Masso-Ferret, E. Nicolau

9:55 Intermission.

10:10 ENFL **102.** Novel carbon nanomaterials for 3rd generation solar cells. **Y.H. Hu**

10:50 ENFL **103.** Small Urbach energies in $CH_3NH_3PbI_{3-x}Br_x$ perovskites that remain constant under degradation. **C.M. Sutter-Fella**, D. Miller, Q. Ngo, E. Roe, F. Toma, I. Sharp, M. Lonergan, A. Javey

11:10 ENFL **104.** Single walled carbon nanotubes in TiO_2 nanofiber photoelectrodes for high performance perovskite and dye-sensitized solar cells. **T.J. Macdonald**, M. Batmunkh, J. Shapter, T. Nann, I.P. Parkin

11:30 ENFL **105.** Silicon nanowires for solar-to-fuel conversion. **Y. Su**, C. Liu, S. Brittman, J. Tang, A. Fu, N. Kornienko, Q. Kong, H. Zhang, P. Yang

11:50 Concluding Remarks.

Section D

Grand Hyatt San Francisco

Curran

Catalysis for Unconventional Energy Sources

Cosponsored by CATL and MPPG²

Y. H. Hu, X. Wang, *Organizers*

S. Chen, X. Fan, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **106.** Reductive disassembly of lignin to fuels and chemicals with porous metal oxide catalysts. **P.C. Ford**, J.A. Barrett, C.M. Bernt, M.A. Chui

9:15 ENFL **107.** Why use sugars to make renewable fuels and materials when the CMF and levulinic acid platforms are one step from raw biomass? **M. Mascal**

9:55 ENFL **108.** Performance of mesoporous alumina supported iron catalyst on Fischer-Tropsch synthesis: Effect of CO_2 and CH_4content in syngas. **S. Badoga**, A.K. Dalai

10:15 Intermission.

10:30 ENFL **109.** Structural engineering of functional nanomaterials for effective electrocatalytic reduction of oxygen. **S. Chen**

11:10 ENFL **110.** Understanding and promoting methane activation using nanocrystal catalysts. **M. Cargnello**, E.D. Goodman, J.H. Maalouf, V.V. Miller, A.R. Riscoe, J.J. Willis, C. Wrasman, L. Wu, A. Yang

11:40 ENFL **111.** CO conversion into liquid hydrocarbons using Co-containing catalyst synthesized in subcritical conditions. **E. Sulman**, A. Stepacheva, A. Gavrilenko, M. Markova, V. Molchanov, M. Sulman

12:00 Concluding Remarks.

Section E

Grand Hyatt San Francisco

Sequoia

Innovative Chemistry & Materials for Electrochemical Energy Storage

Flow Batteries & Organic Electrodes

Cosponsored by MPPG² and PMSE

J. Guo, E. Pomerantseva, *Organizers*

Y. Mo, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **112.** Lithium redox flow battery as an emerging technology for large-scale energy storage. **G. Yu**

9:05 ENFL **113.** Asymmetric sulfonated Diels-Alder poly(phenylene)s: Effect of membrane morphology on vanadium redox flow battery performance. **T.D. Largier**, C.J. Cornelius

9:25 ENFL **114.** Manipulate the chemical composition and substrate nature to push the cycling stability limit of polypyrrole. **T. Liu**, Y. Song, Y. Li, X. Liu

9:45 ENFL **115.** Reaction mechanism of Sb-based negative electrode materials for Na batteries investigated by operando x-ray absorption spectroscopy: What can we really learn? **L. Stievano**, A. Darwiche, M. Sougrati, C. La Fontaine, L. Monconduit

10:05 Intermission.

10:15 ENFL **116.** Selective block polysulfone anion exchange membranes: Electro-transport characterization and performance in vanadium redox flow batteries. **T.D. Largier**, W. Khan, C.J. Cornelius

10:35 ENFL **117.** Sulfur polymers for stable lithium-sulfur batteries. **M. Preefer**, B. Oschmann, R. Seshadri

10:55 ENFL **118.** Organic materials for energy storage: Exploiting steric strain to tune oxidation potentials. **A. Prins**, N.J. Mortimer, D.R. Henton, A. Dumitrascu, T.F. Guarr

11:15 ENFL **119.** Unraveling charge storage in organic radical polymers for battery electrodes. **J.L. Lutkenhaus**, F. Li, S. Wang

11:35 ENFL **120.** Electrochemical swing process for carbon capture using a polymer-based battery. **S. Voskian**, T. Hatton

Section F

Grand Hyatt San Francisco

Cypress

Computations for CO2 Capture, Conversion & Sequestration

Cosponsored by CATL, COMP, GEOC and MPPG²

V. Glezakou, R. Rousseau, *Organizers*

M. Salvalaglio, *Presiding*

8:30 ENFL **121.** Fate of dissolved carbon dioxide in water under extreme conditions. **G.A. Galli**

9:15 ENFL **122.** Polymeric carbon dioxide at high pressures. **S. Scandolo**

9:50 ENFL **123.** Molecular simulations of the reactivity of H_2O-bearing supercritical CO_2 fluids with silicate minerals. **S.N. Kerisit**, E.J. Bylaska, A.R. Felmy, T. Schaef, J. Loring

10:25 Intermission.

10:45 ENFL **124.** Multiscale simulation approaches in the ONETEP linear-scaling DFT program. **C. Skylaris**

11:20 ENFL **125.** Molecular dynamics and possible catalytic chemistry by molten metals or salts. **H. Metiu**, E.W. McFarland, M.J. Gordon, V. Agarwal, D.C. Upham, H.H. Kristoffersen

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG², ORGN and PROF

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Mechanism of Synthesis

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Electrocatalysis for Energy Generation & Storage

Oxygen Evolution

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Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

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Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy

Sponsored by CELL, Cosponsored by ENFL and ENVR

MONDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Belvedere

Advances in Chemistry of Energy & Fuels

Chemical Looping, Cracking & Gasification

D. J. Heldebrant, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **126.** Investigation of unique phase formation for trimetallic copper iron manganese oxygen carrier. **W. Benincosa**, R.V. Siriwardane, H. Tian, J. Riley

1:55 ENFL **127.** Investigation on the reducibility and regenerability of ferrites as oxygen carrier. **Y. Cao**

2:15 ENFL **128.** Reactivity and recyclability of Cu-based oxygen carrier in solid fuels Chemical Looping with Oxygen Uncoupling (CLOU). **P. Wang**, B.H. Howard, N. Means, D. Shekhawat, D. Berry

2:35 ENFL **129.** Kinetic analysis of the interactions between calcium ferrite and coal char for chemical looping gasification applications: Identifying reduction routes and modes of oxygen transfer. **J. Riley**, R.V. Siriwardane, H. Tian, W. Benincosa

2:55 Intermission.

3:00 ENFL **130.** Behavior and catalytic effects of alkaline metals during co-gasification of coal and biomass. X. Ran, J. Feng, **W. Li**

3:20 ENFL **131.** Exploration on the mechanism of deacidification during catalytic cracking of high acidic crude. **X. Wei**, A. Mao

3:40 ENFL **132.** Design and synthesis of Vanadium-Titanium-incorporated Mesoporous Silica (VTi/MCF) catalysts for the oxidative dehydrogenation of propane to propylene. **Z. Xie**, **Z. Zhao**

4:00 Concluding Remarks.

Section B

Grand Hyatt San Francisco
Filmore C

C1 Catalysis

Cosponsored by CATL

K. Ding, *Organizer*

N. Kumar, J. J. Spivey, *Organizers*, *Presiding*

1:30 ENFL **133.** Natural gas conversion to higher-value products: Challenges and opportunities. **J.J. Spivey**, Z. Wang, S. Kanitkar, N. Kumar, D. Berry, D. Shekhawat, D. Haynes

2:10 ENFL **134.** Co_2C nanostructures with facet effect for Fischer-Tropsch to olefins. F. Yu, Y. An, Z. Li, **L. Zhong**, **Y. Sun**

2:30 ENFL **135.** Metal organic framework-mediated synthesis of cobalt catalysts for higher oxygenates synthesis. **Z. Wang**, G. Laddha, S. Kanitkar, **J.J. Spivey**

2:50 ENFL **136.** Elucidating the nature of Fe species during pyrolysis of the Fe-BTC MOF into highly active and stable Fischer–Tropsch catalysts. **T. Wezendonk**, M. Makkee, F. Kapteijn, J. Gascon

3:10 Intermission.

3:25 ENFL **137.** Selective formation of long-chain hydrocarbons from CO_2 hydrogenation over TiO_2 supported Co-Cu-K catalysts. Z. Shi, **P. Gao**, S. Dang, L. Zhong, **H. Wang**, Y. Sun

3:45 ENFL **138.** CO_2 electrocatalytic and photoelectrocatalytic conversion for oxygenate synthesis. **W. Chen**, X. Bai, R. Ge, W. Wei, Y. Sun

4:05 ENFL **139.** Electronic structure tuned electrochemical CO_2 reduction on silver-based electrodes. **Z. Wang**, J. Zhou

4:25 ENFL **140.** CO_2-utilized chemical looping reforming with phase transition of Fe_2O_3–NiO to $NiFe_2O_4$ in perovskite catalysts. J.W. Lee, **D. Kang**, **H. Lim**

4:45 Concluding Remarks.

Section C

Grand Hyatt San Francisco
Orpheum

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Cosponsored by CATL, MPPG‡ and PMSE

R. T. Koodali, H. Wang, *Organizers*

Y. H. Hu, *Organizer, Presiding*

J. Z. Zhang, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **141.** Origin of instability and surface chemistry approach to stabilization of organ-metal halide perovskites. **J.Z. Zhang**

2:15 ENFL **142.** Picosecond light-induced rotational disordering in the hybrid perovskites. **A. Lindenberg**

2:45 ENFL **143.** Multiscale patterned photoelectrodes for enhanced light harvesting in mesoscopic solar cells. **J. Kang**, S. Jang, Y. Son, A. Lim, J. Kim, J. Jeong, M. Choi, Y. Sung

3:05 ENFL **144.** Phase change capsule with water-absorbable polymeric shell for thermal energy storage and delivery. **T. Do**, Y. Ko, U. Choi

3:25 Intermission.

3:40 ENFL **145.** Overcoming the mechanical fragility of perovskite solar cells using novel cross-linking chemical additives and scaffolds. **B. Watson**, N. Rolston, K. Bush, A. Printz, R. Dauskardt

4:00 ENFL **146.** Exploring highly efficient hydrogen peroxide generation on reduced graphene oxide electrocatalysts. **H. Kim**, B.D. McCloskey

4:20 ENFL **147.** Nanostructured promoted titania photocatalysts for solar fuels. **R. Trofimovaite**, C.M. Parlett, M. Isaacs, S. Kumar, A.F. Lee

4:40 ENFL **148.** Hybrid organic-inorganic quantum dot superlattices for photovoltaics. **D. Yang**, Z. Guan, M. Law, A. Abelson

5:00 ENFL **149.** Tailored annealing and surface treatment of Bi_2S_3 thin film to enhance optoelectronic performance. **Z. Zhu**, S. Iyemperumal, A.D. Carl, L. Zhou, R. Grimm, N.A. Deskins, P. Rao

5:20 Concluding Remarks.

Section D

Grand Hyatt San Francisco
Curran

ENFL Distinguished Researcher Award: Symposium in honor of Mieczyslaw M. Boduszynski

C. F. Ovalles, *Organizer*

M. M. Boduszynski, M. Moir, *Organizers*, *Presiding*

C. Ovalles, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **150.** Do asphaltenes really exist? **M. Moir**

2:05 ENFL **151.** Confirmation of the Boduszynski continuum by high-resolution Fourier transform ion cyclotron resonance mass spectrometry. **R.P. Rodgers**, Y. Corilo, D.C. Podgorski, S. Rowland, P.M. Lalli, A.C. Clingenpeel, J. Lu, A.G. Marshall

2:35 ENFL **152.** Equivalent distillation: Examining the properties of non-distillable materials in crude oils. **E. Rogel**, J. Vien, M. Roye, T. Miao

3:05 Intermission.

3:25 ENFL **153.** Compatibility of heavy oils and bitumen. Blending, refining and upgrading. **P. Rahimi**

3:55 ENFL **154.** Insights from Dr. M. M. Boduszynski that influenced research on instrumental induced thermal cracking and large paraffins' existence. **L.A. Carbognani**

4:25 ENFL **155.** From a dream to a fact: Direct measurement of vanadium and nickel distribution on VGO's. **F.A. Lopez-Linares**, M.M. Boduszynski, C.E. Rechsteiner, M. Moir, D. Leong, L. Poirier, J. Nelson

4:55 ENFL **156.** Preparative separation of petroleum residua and asphaltene fractions using inert supports. Mietek's pioneer work. **C.F. Ovalles**, E. Rogel, M. Moir

5:25 Concluding Remarks.

Section E

Grand Hyatt San Francisco
Sequoia

Innovative Chemistry & Materials for Electrochemical Energy Storage

Capacitors

Cosponsored by MPPG‡ and PMSE

J. Guo, Y. Mo, *Organizers*

E. Pomerantseva, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **157.** Development of pseudocapacitance in oxide materials. **B. Dunn**

2:05 ENFL **158.** MnO and MnNCN for Li-ion capacitors. **G. Cao**

2:35 ENFL **159.** Understanding supercapacitor by joint density functional theory. **C. Zhan**, Y. Zhang, P.T. Cummings, D. Jiang

2:55 ENFL **160.** Highly-integrated and flexible 3D supercapacitors prepared with vertically aligned CNTs and reconfigurable solid state electrolyte films. **H. Kim**, S. Hong, R. Lavall, Y. Jung

3:15 ENFL **161.** 3-Dimensional nonwoven and textile substrates associated with iridium oxide nanoparticles for the improvement of specific capacitance. **S. McGraw**, K. Chow, D. Wickramasinghe, R. Czerw, K. Senecal

3:35 Intermission.

3:45 ENFL **162.** Improving the capacitance of graphene aerogel electrodes via a facile ion-intercalation strategy. **T. Liu**, C. Zhu, M.A. Worsley, Y. Li

4:05 ENFL **163.** Fabrication of an advanced, high-performance all-solid-state asymmetric supercapacitor with polypyrrole wrapped cobalt vanadium oxide hydrate as positive and graphene nanoplatelets as negative electrode for power device applications. **A. Maitra**, B.B. Khatua

4:25 ENFL **164.** Facilitated charge transport in PANI/α-$Ni(OH)_2$/iron oxide doped reduced graphene oxide composite based hybrid pseudocapacitive electrode material for supercapacitor with excellent power characteristics. **A.K. Das**

4:45 ENFL **165.** On the double layer capacitance of graphite. **H. Liu**

5:05 ENFL **166.** Nickel tungstate nanoparticles decorated reduced graphene oxide nanocomposite as anode material for Li-ion battery. **R. Kumar**

Section F

Grand Hyatt San Francisco
Cypress

Computations for CO2 Capture, Conversion & Sequestration

Cosponsored by CATL, COMP, GEOC and MPPG‡

V. Glezakou, R. Rousseau, *Organizers*

S. N. Kerisit, *Presiding*

1:30 ENFL **167.** Interactions of CO_2 with metal oxide nanoclusters, metal organic frameworks, and clays. L. Flores, K.S. Thanthiriwatte, J.G. Murphy, W.B. Copeland, **D.A. Dixon**

2:05 ENFL **168.** Computational studies of electrochemical reduction of CO_2 to CO using transition metal dichalcogenide nanoflakes. **C. Liu**, L.A. Curtiss

2:30 ENFL **169.** CO_2 activation employing a silylium–phosphine frustrated Lewis pair. **P. Hunt**

3:05 Intermission.

3:25 ENFL **170.** Tuning activity and selectivity toward CO_2 conversion: Going from metal, metal alloy to metal-oxide. S. Kattel, B. Yan, J.G. Chen, J. Rodriguez, **P. Liu**

4:00 ENFL **171.** Regulation of the redox properties of tungsten-alkylidyne complexes by ligand design. **B. Rudshteyn**, H.B. Vibbert, R. May, E. Wasserman, I. Warnke, M.D. Hopkins, V.S. Batista

4:25 ENFL **172.** Nitrogenase reduction of N_2 and CO_2. **S. Raugei**, L.C. Seefeldt, B.M. Hoffman

Section G

Moscone Center
Halls B/C

Advances in Chemistry of Energy & Fuels

D. J. Heldebrant, S. J. Riley, *Organizers*

2:00 - 4:00

ENFL **173.** Application of the immobilized lipase on graphene oxide/$Zn_xFe_{1-x}Fe_2O_4$ composite nanoparticles to produce biodiesel in nonaqueous media. **R.K. Sharma**, N. Kumar, C.A. O'Neill, K. Gaur, M. Saxena, G. Morell, K. Griebenow

ENFL **174.** Integrated electrochemical-biological systems for the production of fuels and chemicals from CO_2. **A.D. Antoniuk-Pablant**, F. Kracke, J. Deutzmann, T.F. Jaramillo, A. Spormann

ENFL **175.** High performance terpenoid biofuel production by oleaginous yeast *Rhodosporidium toruloides*. **X. Zhuang**

ENFL **176.** Production of biodiesel from vegetable oil. **V. Martinez**, G.C. Peña

ENFL **177.** Lipid analyses of assembled and naturally occurring algal communities cultivated in agricultural wastewater. **A.R. Good**, P.K. Thomas, G.P. Dunn, K. Feris, M.P. Callahan

ENFL **178.** Withdrawn.

ENFL **179.** Withdrawn.

‡ *Cooperative Cosponsorship*

ENFL **180.** Simultaneous production of biodiesel and valuable co-products from *in-situ* transesterification of wet microalgae. H. Im, **J. Park**, B. Kim, J.W. Lee

ENFL **181.** Tremella-like N,O-codoped hierarchical porous carbon nanosheets derived from cattle bone for fast and stable sodium storage. **J. Niu**, J. Liang, R. Shao, M. Dou, F. Wang

ENFL **182.** Analysis of oxygenates in bio-oils. **A.B. Padmaperuma**, M.V. Olarte, T. Lemmon, M. Swita, S.D. Burton, B.A. Hofstad

ENFL **183.** Production, blending, and upgrading of advanced renewable fuels for the co-optimization of fuels and engines. **E. Monroe**, R.W. Davis, A. George, J.M. Gladden

ENFL **184.** Enhancement of methane production by varying operating conditions in anaerobic digesters fed with cow manure and barley. B. Tutal, **Ç. Akyol**, O. Ince, E. Ozbayram, P. Kurt Polat, K. Yagdi, B. Ince

ENFL **185.** Effects of alkylamine electrolyte additives on activity and selectivity in electrochemical carbon dioxide reduction. **J. Lin**, C. Hahn, T.F. Jaramillo

ENFL **186.** Mechanism of CO_2 reduction monitored by rapid-scan FT-IR spectroscopy on two different catalysts: Cobalt(II) tetraaza macrocyclic complexes and copper nanoparticles. **H. Sheng**, H.M. Frei

ENFL **187.** Effects of the performance of hydrogen selective membrane for CO_2 capture on the techno-economics of integrated gasification combined cycle. **G. Lee**, J. Park, K. Hwang, J. Park, M. Park

ENFL **188.** Waste and cost reduction by reprocessing used motor oil into a synthetic diesel fuel. **J.K. Shurtleff**

ENFL **189.** High resolution mass spectrometric analysis of crude oil vacuum resid and its chromatographically separated fractions using an orbitrap mass spectrometer. **M. Hurt**

ENFL **190.** Perspective of methane hydrate formation kinetics with promoters: A perspective of methane hydrate formation kinetics with promoters. **P. Rangsunvigit**, A. Siangsai, K. Inkong, S. Kulprathipanja

ENFL **191.** Study on the origin of corrosive hydrogen chloride in crude oil distillation from the viewpoint of organic chlorides. **B. Wu**, J. Zhu, R. Ma

ENFL **192.** Functionalization of asphaltenes by acid treatment. **M.N. Siddiqui**

ENFL **193.** Pitch-based nitrogen-doped mesoporous carbon for flue gas desulfurization. **X. Song**

ENFL **194.** Influence of ensemble and ligand effects of PdAU catalyst on formic acid dehydrogenation: Experimental and computational studies. **C. Yoon**, H. Ham

ENFL **195.** Formic acid dehydrogentation over PdNi alloy catalysts: Experiments and theoretical investigation. **C. Yoon**, D. Lim, R. Tamarany

ENFL **196.** Developing catalysts and methods for low temperature electrochemical oxidation of methane. **M.J. Boyd**, C. Hahn, T.F. Jaramillo

ENFL **197.** Hydrodesulfurization of dibenzothiophene using lanthanum doped CoMoS2 catalysts. **C. Valdes**, D.F. Gonzalez, J.G. Parsons

ENFL **198.** CeO_2/graphene and Nb_2O_5/graphene supported Pt and PtCo catalysts towards methanol and ethanol oxidation and oxygen reduction reactions. **V. Kepeniene**, L. Tamasauskaite Tamasiunaite, A. Selskis, E. Norkus

ENFL **199.** Gas agents effect of co-gasification of coal and biomass on alkali metal migration and its catalytic performance. L. Wang, J. Feng, **W. Li**

ENFL **200.** Catalytic methane decomposition and oxidative regeneration by CO_2 over nickel-carbon core-shell catalyst. J.W. Lee, D. Kang, **H. Lim**

ENFL **201.** Structural and elemental influence of various MOFs on the performance of Fe@C catalysts for Fischer-Tropsch synthesis. **T. Wezendonk**, M. Makkee, F. Kapteijn, J. Gascon

ENFL **202.** High-performance hydrogen evolution from $MoS_{2(1-x)}P_x$ solid solution. **R. Ye**, Y. Liu, M.J. Yacaman, B.I. Yakobson, J.M. Tour

ENFL **203.** Adsorption and dehydrogenation of ethane, propane and butane on Rh_{13} clusters supported on unzipped graphene oxide and TiO_2(110): A DFT study. **C. Chang**, **M. Tsai**

ENFL **204.** Synthesis of mesoporous silica-supported and size-constrained bismuth vanadate for photocatalytic oxygen evolution and environmental remediation applications. **D. Harts**

ENFL **205.** Earth-abundant nickel-iron hybrid catalysts for solar fuels production. **B. Weintraub**

ENFL **206.** Activation and stabilization of copper chalcopyrite light absorbers for photoelectrochemical hydrogen production. **D. Palm**, T. Hellstern, A. DeAngelis, N. Gaillard, T.F. Jaramillo

ENFL **207.** Polyvinyl chloride and cubic $ZnSnO_3$ nanoparticles based nanocomposite as high output power and durable piezoelectric nanogenerator. **S. Paria**

ENFL **208.** Vanadium-doped zinc oxide nanosheets-polymer composite for piezoelectric energy harvesting. **J. Nah**, S. Shin, Y. Kwon, M. Lee

ENFL **209.** Synthesis and application of freestanding 3D Fe-coordinated nitrogen doped carbon for energy storage and Oxygen Reduction Reaction (ORR) using iron doped poly(1,8-diaminonaphthalene) precursor. **C. Ortuno-Quintana**, K. Ramirez, J. Lu

ENFL **210.** Electrochemical behavior of shape controlled Pt-Rh nanoparticles for ammonia oxidation in alkaline medium for direct alkaline fuel cell application. **R.A. Martinez-Rodriguez**, F.J. Vidal-Iglesias, J. Solla-Gullón, C.R. Cabrera, J.M. Feliu

ENFL **211.** Withdrawn.

ENFL **212.** Desymmetrized bay-annulated indigo donor-acceptor materials: Methodology, self-assembly, and use in organic electronics. **M. Kolaczkowski**, B. He, M. Roders, A. Ayzner, Y. Liu

ENFL **213.** Highly efficient radial-junction microwire solar cells by acid based doping process. **I. Hwang**, K. Seo

ENFL **214.** Fabrication of ceramic selective emitter for a thermophotovoltaic system with enhanced efficiency. **K. Park**, J. Kim, D. Kim, Y. Kim

ENFL **215.** Organic photovoltaic properties of 6-(2-thienyl)-4H-thieno[3,2-b]indole based conjugated polymers containing fluorinated benzothiadiazole. **A. Yi**, S. Chae, I. Jeong, J. Kim, H. Suh, H. Kim

ENFL **216.** Nanostructured tungsten carbide for Pt-free counter electrode of dye-sensitized solar cells. **J. Kim**, J. Kang, M. Lee, Y. Son, J. Jeong, A. Lim, H. Park, Y. Sung

ENFL **217.** Fabrication of cobalt oxides embedded carbon nanofibers for high performance energy storage devices. **C. Ranaweera**, C. Zhang, S. Bhoyate, A. Jimenez, P.K. Kahol, R. Gupta

ENFL **218.** Improving performance of 2-cyanoethyltrimethoxysilane (CNETMS)-based capacitors through the incorporation of charge blocking layers. **Y. Park**, M. Kathaperumal, J.W. Perry

ENFL **219.** Flexible energy storage device based on nanostructured cobalt sulfide. S. Aloqayli, C. Ranaweera, Z. Wang, P.K. Kahol, **K.S. Siam**, R. Gupta

ENFL **220.** Vanadium hexacyanoferrates Prussian blue analogues for multiple-redox enabled high performance aqueous rechargeable batteries. J. Lee, G. Ali, D. Kim, H. Jung, **K. Chung**

ENFL **221.** Synchrotron-based x-ray diffraction study on the effect of cobalt substitution in the electrochemical performance of $NaFeO_2$ as a cathode material for Na-ion batteries. D. Susanto, G. Ali, W. Choi, W. Chang, **K. Chung**

ENFL **222.** Perfluorinated anion-based single-ion conducting polymers. **I. Popovs**, X. Sun, S. Dai

ENFL **223.** Effect of TiO_2 morphology @ Ti foam anode on the performance of lithium ion battery. **K. Nam**, H. Choe

ENFL **224.** High energy capacity flexible lithium-ion batteries using silicon particle anode. **J. Im**, **K. Cho**, S. Yoon, E. Hwang, Y. Kwon, Y. Lee, J. Ahn

ENFL **225.** Application of PEG-based solid polymer electrolyte to all-solid-state Li-O_2 batteries. **S. Cho**, J. Yom, W. Yoon

ENFL **226.** Improvement of cycling performances of high-voltage lithium-ion battery using fluorinated functional additives. **J. Im**, J. Ahn, K. Cho, S. Yoon, E. Hwang, Y. Kwon

ENFL **227.** Wearable fibrous lithium ion batteries. **S. Ha**, G. Lee, C. Lee, S. Kim, Y. Lee

ENFL **228.** Kinetic analysis of irreversible behavior in silicon monoxide anode by GITT, EIS and CV for lithium ion battery. **J. Yom**, S. Cho, W. Yoon

ENFL **229.** Solid polymer electrolytes for multifunctional material systems. **W. Andrews**, C.C. Browder

ENFL **230.** Li_8ZrO_6: A cathode material for lithium-ion batteries. **Y.E. Chipangura**, A. Stein, N. Tran

ENFL **231.** Carbon nanofibers as current collector for Li/deep eutectic catholyte battery system. **K. Kawase**, J. Abe, Y. Kobayashi, S. Shiratori

ENFL **232.** SnO_2 nanoneedle@carbon nanofiber composite material as self-standing anode material for lithium-ion batteries. **K. Takahashi**, J. Abe, K. Kawase, Y. Kobayashi, S. Shiratori

ENFL **233.** Morphology and electrochemical property of carbon/iron oxide composites fabricated by electrodeposition. **Y. Kobayashi**, J. Abe, K. Kawase, K. Takahashi, S. Shiratori

ENFL **234.** Sub-10-nm Co_3O_4 nanoparticles/graphene composites as high-capacity anodes for lithium ion batteries. **K. Jang**, J. Jang, H. Song, K. Cho, F. Auxilia, M. Ham

ENFL **235.** Ether and siloxane functional ILs in propylene carbonate for Li-ion batteries. **S.N. Chavan**, D. Mandal

ENFL **236.** Etching of aluminum cathode current collector and its electrochemical properties for Li-ion batteries. **S. Yoon**, K. Cho

ENFL **237.** Electrochemical characteristics of the self-standing iron oxide/carbon composite electrospun nanofibers. **J. Abe**, K. Kawase, S. Shiratori

ENFL **238.** Computational experiments on drivers of Li^+ diffusion using lithium-oxyhalide anti-perovskites. **Z. Mehmedović**, N. Adelstein

ENFL **239.** Simplified correlation equations for density, transport, and thermal properties of supercritical carbon dioxide in geothermal heat extraction and carbon sequestration applications. **P.X. Tran**, M. Massoudi, **P. Wang**, M.L. McKoy

ENFL **240.** First-principles calculations of thermoelectric properties of Bi_2Te_3 and PbTe. H. Kim, G. Choi, M. Ha, **W. Lee**

ENFL **241.** Development of a kinetic model for the hydrodechlorination of trichloromethane over Pt-Pd/KIT-6. **M. Son**, S. Sung, S. Lee, J. Cho, S. Kim, J. Bae, M. Park

Rising Star Award Symposium

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MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

D. J. Heldebrant, *Organizer*

8:00 - 10:00

23, 27, 48, 54, 57, 82, 96, 98-99, 104-105, 107, 117, 120, 126, 165, 174, 183, 186. See previous listings.

242, 271, 275, 279, 286-287, 293, 294, 300, 316, 327, 333, 340, 358, 367, 381, 398, 410, 412, 421, 442, 446-447, 455. See subsequent listings.

TUESDAY MORNING

Section A

Grand Hyatt San Francisco
Belvedere

Advances in Chemistry of Energy & Fuels

Fuel Cells, Photocatalysts & Hydrogen

D. J. Heldebrant, *Organizer*

Z. Li, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **242.** Catalytic hydrogen generation from formic acid and its subsequent utilization to produce electricity: An indirect formic acid fuel cell. **M. Czaun**, A. Goeppert, B. Yang, J. Kothandaraman, S. Greenberg, S.G. Prakash, G. Olah

8:55 ENFL **243.** Withdrawn.

9:15 ENFL **244.** Synthesis of bio-inspired covalently functionalized graphene nanohybrid and comparison of the effect of different electron transfer pathway on the photocatalytic hydrogen production efficiency. **J. Yan**

9:35 ENFL **245.** Ligand engineering of lead chalcogenide nanoparticle solar cells. **M. Voros**, N.P. Brawand, G.A. Galli

9:55 ENFL **246.** Effect of geometrical site confinement in high-efficient iron-doped cobalt oxides electrocatalysts toward oxygen evolution reaction. **S. Hong**, Y. Hsu, H. Chen

10:15 ENFL **247.** Superior performance of borocarbonitrides, $B_x C_y N_z$, as stable, low-cost metal-free electrocatalysts for the hydrogen evolution reaction. **H. Chakraborty**, M. Chhetri, S. Maitra, U. Waghmare, C. Rao

10:35 Intermission.

10:40 ENFL **248.** Molecular modeling of activated carbon-based electrochemical double layer capacitors. S. Schweizer, **L. Subramanian**, J. Hill

11:00 ENFL **249.** Exploration of inorganic and hybrid porous materials as proton conductors. **S. Devautour-Vinot**, P. Mileo, D. Damanesco Borges, R. Semino, G. Maurin, F. Paesani, H. Jobic, N. Stenou, F. Nouar, C. Serre

11:20 ENFL **250.** Nanoporous Sn and SbSn anode for Li and Na ion batteries through one-step selective etching. **T.C. Lin**, J.B. Cook, E. Detsi, J. Weker, S.H. Tolbert

11:40 ENFL **251.** Inkjet printing assisted fabrication of hierarchical Ni@ MnO2 dendritic nanostructured electrode for flexible micro-supercapacitor with artistic design. **Y. Lin**, Y. Gao, Z. Fan

12:00 ENFL **252.** Open porous hierarchical SiC@nanographene@phosphorus structure and its electrochemical performance as a Li-ion anode. **D. Zhao**, B. Li, J. Zhang, C. Niu

12:20 Concluding Remarks.

Section B

Grand Hyatt San Francisco
Filmore C

Functional Porous Materials for Sustainable Energy

Cosponsored by CATL and MPPG‡

N. L. Rosi, S. Shanmugam, *Organizers*

R. Motkuri, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **253.** Reticular materials for clean energy and water. **O.M. Yaghi**

9:05 ENFL **254.** Single site catalysis in metal-organic frameworks. **C.J. Doonan**, A. Burgun, C. Sumby

9:25 ENFL **255.** Metal organic frameworks: Functional porous materials for energy-efficient and selective gas capture and separation. B. Li, H. Wang, **J. Li**

9:45 ENFL **256.** Encapsulation of bio-catalysts into nanoporous materials. **C. Tsung**

10:05 Intermission.

10:15 ENFL **257.** Metal-organic frameworks for artificial photosynthesis. **W. Lin**

10:35 ENFL **258.** Metal organic framework derived, nitrogen doped carbon for high stability room temperature sodium-sulfur battery. **Y. Zhu**

10:55 ENFL **259.** First principles-based computational design concept for highly functional materials for energy systems. **B. Han**

11:15 ENFL **260.** Fundamentals and applications of electrically conductive two-dimensional MOFs. **M. Dinca**, D. Sheberla, L. Sun, M. Campbell, E. Miner

11:35 Concluding Remarks.

Section C

Grand Hyatt San Francisco
Orpheum

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Cosponsored by CATL, MPPG‡ and PMSE

R. T. Koodali, H. Wang, *Organizers*

Y. H. Hu, *Organizer, Presiding*

Z. Wu, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **261.** Exploring two-dimensional materials as novel photocatalysts for hydrogen production from water splitting. **Z. Wu**

9:15 ENFL **262.** Exploring new opportunities in organic-inorganic hybrid perovskites. **T. Xu**

9:45 ENFL **263.** Thin films of methylammonium lead halide perovskite via hydrolysis of N-methylformamide as source of methylammonium ions. **S. Accornero**, M. Arciniegas, M. Prato, S. Marras, L. Manna

10:05 ENFL **264.** Efficient TiO_2 thin films prepared via adsorptive self-assembly for photovoltaic self-cleaning and anti-soiling applications. **R. Isaifan**, T. Rhadfi, A. Samara, B. Aissa, A. Abdallah

10:25 ENFL **265.** Phase-stabilized α-$CsPbI_3$ quantum dots and fabrication of all-inorganic perovskite devices. **A. Marshall**, A. Swarnkar, E. Sanehira, J. Luther

10:45 Intermission.

11:00 ENFL **266.** 2D layer as a protection against film degradation on perovskite solar cells. **M.S. Holanda**, A. Nogueira

11:20 ENFL **267.** Dense silica barrier films for improved efficiency and stability of perovskite solar cells deposited in ambient air. **N. Rolston**, A. Printz, S. Dong, B. Watson, R. Dauskardt

11:40 ENFL **268.** Flexible crystalline silicon photovoltaics with vertically aligned microwire array. **I. Hwang**, H. Um, K. Seo

12:00 ENFL **269.** Neutral-color semi-transparent crystalline silicon solar cells. **K. Lee**, N. Kim, H. Um, I. Hwang, K. Seo

12:20 Concluding Remarks.

Section D

Grand Hyatt San Francisco
Curran

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Catalysis

Cosponsored by ANYL

K. Herwig, *Organizer*

R. E. Winans, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **270.** Characterization of Pt/C during electrocatalytic hydrogen addition reactions. **J. Fulton**, N. Singh, D.M. Camaioni, N. Govind, D.C. Cantu, R. Rousseau, M. Balasubramanian, S. Russell, C.T. Campbell, J.A. Lercher

9:05 ENFL **271.** Following chemistry and catalysis in metal-organic frameworks using advanced synchrotron x-ray scattering tools. **A. Platero Prats**, K.W. Chapman, D.M. Camaioni, C.J. Cramer, O.K. Farha, J. Fulton, L. Gagliardi, J.T. Hupp, C. Lu, A.B. Martinson, A. Stein, D.G. Truhlar

9:35 ENFL **272.** VISION challenge: The world's first high-throughput inelastic neutron scattering spectrometer. **A. Ramirez-Cuesta**, Y. Cheng, L. Daemen

10:05 Intermission.

10:20 ENFL **273.** Investigation on catalytic metal nanoparticle synthesis. **H. Zhao**, Y. Lei

10:50 ENFL **274.** *In situ* isotope-contrasted stroboscopic studies of the local atomistic structure of catalytic materials. D. Olds, K. Page, A. Päcklar, P. Peterson, **J.R. Neilson**

11:20 ENFL **275.** Characterizing the local structure and reactivity of nanoscale catalysts through combined x-ray scattering and vibrational spectroscopy measurements. **P. Chupas**

11:50 Concluding Remarks.

Section E

Grand Hyatt San Francisco
Sequoia

Innovative Chemistry & Materials for Electrochemical Energy Storage

Solid-State Electrolytes & Beyond Li

Cosponsored by MPPG‡ and PMSE

J. Guo, Y. Mo, *Organizers*

E. Pomerantseva, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **276.** Quest for novel electrolytes - Challenges and opportunities. **S. Meng**

9:05 ENFL **277.** Stability and cycling of metallic lithium with an inorganic solid electrolyte. **N.J. Dudney**, M. Chi, E. Herbert, J. Sakamoto

9:35 ENFL **278.** Novel alkali superionic conductor solid electrolytes. **S. Ong**, Z. Zhu, I. Chu

10:05 ENFL **279.** 3D all solid state Li-ion microbatteries. **A. Talin**

10:35 Intermission.

10:45 ENFL **280.** Understanding Li^+ diffusion behavior in amorphous and crystalline Li_3PS_4 solid electrolytes, via *ab-initio* simulations. **N. Leclerc**, N. Adelstein

11:05 ENFL **281.** Aluminum triflate in diglyme: A potential electrolyte for Al-ion batteries. **E.J. Menke**, L. Reed, A. Arteaga

11:25 ENFL **282.** Synthesis of a magnesium battery electrolyte without need for conditioning or promoters. **T. Hou**, C.W. Monroe

11:45 ENFL **283.** Fundamental investigations of magnesium electrode/electrolyte interface using *operando* ambient pressure x-ray photoelectron spectroscopy. **Y. Yu**, A. Baskin, C. Valero-Vidal, N. Hahn, K.R. Zavadil, B.W. Eichhorn, D. Prendergast, E.J. Crumlin

12:05 ENFL **284.** Sodium electrolyte degradation: Evaluating pure electrolyte degradation through a safe and convenient NMR technique. **P.L. Barnes**, H. Xiong, K. Smith, E.J. Dufek

Section F

Grand Hyatt San Francisco
Cypress

Biomass & Biofuel Processing

Cosponsored by CELL, MPPG‡ and WCC

J. Fu, S. Turn, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **285.** Demonstration of fast pyrolysis technologies at pilot-scale. **E. Wilcox**, T. Dunning

8:55 ENFL **286.** Fast pyrolysis: Comparing effects of feedstock and run conditions on fast pyrolysis products produced at the pilot scale. **T. Dunning**, E. Wilcox

9:15 ENFL **287.** Lignocol: Low ash, low sulfur coal replacement from fast pyrolysis of biomass. **M.R. Rover**, A. Friend, R.G. Smith, R.C. Brown

9:35 ENFL **288.** Ex-situ catalytic fast pyrolysis in a DCR – Effect of pyrolysis conditions. **M. Jarvis**, J. Olstad, Y. Parent, K.A. Magrini

9:55 Intermission.

10:10 ENFL **289.** Upgrading biomass pyrolysis vapors to fungible hydrocarbon intermediates. **K.A. Magrini**, M. Jarvis, J. Olstad, Y. Parent, S. Deutch, M. Yung, K. Iisa

‡*Cooperative Cosponsorship*

10:30 ENFL **290.** Recovering and upgrading biogenic carbon from pyrolysis waste streams to produce chemical intermediates. **C. Mukarakate**, A. Starace, R.J. Evans, K.A. Magrini

10:50 ENFL **291.** Biofuel production by catalytic pyrolysis vapor upgrading: Effects of nickel loading and pretreatment on modified ZSM-5. **M. Yung**, A. Starace, C. Mukarakate, K.A. Magrini

11:10 ENFL **292.** Constant volume pyrolysis of biomass for the production of char with high fixed-carbon content. **M. Legarra Arizaleta**, S. Van Wesenbeeck, S. Turn, T.J. Morgan

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

Carbohydrate Processing & Upgrading of Biomass-Derived Molecules

Sponsored by CATL, Cosponsored by CARB and ENFL

Cellulose Structure & Biosynthesis

Biochemistry & Cellular Biology

Sponsored by CELL, Cosponsored by BIOL, BIOT, CARB and ENFL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Molecular & Bio-Inspired Photocatalysts

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

TUESDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Belvedere

Advances in Chemistry of Energy & Fuels

Batteries

D. J. Heldebrant, *Organizer*

Z. Li, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **293.** First-principles molecular dynamics of non-arrhenius Li^+ diffusion in solid electrolytes for batteries. **A. Zevgolis**, N. Adelstein

1:55 ENFL **294.** Nanoporous $LiMn_2O_4$: An extrinsically pseudocapacitive cathode material for Li-ion batteries. **B. Lesel**, J. Ko, J.B. Cook, Y. Yan, B. Dunn, S.H. Tolbert

2:15 ENFL **295.** Electrochemical activation and reduction of SF_6 in nonaqueous Li cells for primary energy delivery. **B. Gallant**, Y. Li

2:35 ENFL **296.** Withdrawn.

2:55 Intermission.

3:05 ENFL **297.** Withdrawn.

3:25 ENFL **298.** Large-scale preparation of redox active organics for symmetric nonaqueous redox flow batteries. **J. Saraidaridis**, R. Straker, C.S. Sevov, J. Suttil, M.S. Sanford, M.C. Willis, C.W. Monroe

3:45 ENFL **299.** Self-healing polymer for high capacity anodes. **C. Wang**

4:05 ENFL **300.** Effect of ion stabilization and thermal annealing on cycling behavior of bilayered vanadium oxides in Na-ion batteries. **M. Clites**, E. Pomerantseva

4:25 ENFL **301.** Morphology tailored porous hollow Cu_2O nanospheres fabricated by Ostwald ripening for Li-ion battery applications. **P. Rai**, S. Shilpa, A. Sharma

4:45 Concluding Remarks.

Section B

Grand Hyatt San Francisco
Filmore C

Functional Porous Materials for Sustainable Energy

Cosponsored by CATL and MPPG‡

R. Motkuri, S. Shanmugam, *Organizers*

N. L. Rosi, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **302.** Design and synthesis of amine-functionalized porous materials for carbon capture. Y. Sun, **H. Zhou**

2:00 ENFL **303.** Metal organic frameworks for carbon activation and conversion. **A.J. Morris**, J. Zhu, P. Usov

2:20 ENFL **304.** Diamine-appended metal-organic frameworks as cooperative adsorbents for energy-efficient CO2 separations. **J. Martell**, P.J. Milner, R.L. Siegelman, J.R. Long

2:40 ENFL **305.** Withdrawn.

3:00 Intermission.

3:10 ENFL **306.** Functional Metal-Organic Frameworks (MOFs): Design and preparation. **O.K. Farha**

3:30 ENFL **307.** Amine functionalized porous polymer microspheres for enhanced CO_2 capture. N.A. Dogan, E. Ozdemir, **C.T. Yavuz**

3:50 ENFL **308.** Porous materials for capture of fluorinated species. **O. Miljanic**

4:10 ENFL **309.** Production of stable metal organic heat carrier nanofluids. **S.K. Nune**, P. McGrail, M. Nandasiri, J. Jenks, N. Phillips

4:30 Concluding Remarks.

Section C

Grand Hyatt San Francisco
Orpheum

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Cosponsored by CATL, MPPG‡ and PMSE

R. T. Koodali, H. Wang, *Organizers*

Y. H. Hu, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **310.** Withdrawn.

2:15 ENFL **311.** Ionic-liquid electrolyte solidified by surface modified nanoparticles for dye-sensitized solar cells. **Y. Lin**, Y. Fang, P. Ma

2:35 ENFL **312.** Rapid microwave-hydrothermal synthesis of TiO_2-MgO for photocatalytic energy and environmental remediation applications. **B. Selvaratnam**, R.T. Koodali

2:55 ENFL **313.** Effect of ligands on photochemical charge transfer in CdSe quantum dot films – A surface photovoltage spectroscopy study. **B. Nail**, M.J. Greaney, H. Lu, J. Zhao, S.E. Bradforth, R.L. Brutchey, F.E. Osterloh

3:15 Intermission.

3:30 ENFL **314.** Thin film upconversion sensitized by zinc-blende CdSe nanocrystals. **J. Tamayo**, L. Chen, J.J. Locklin, P. Xia, M. Tang

3:50 ENFL **315.** Solar energy harvesting scheme utilizing low dimensional micro- and nano-structures. **Y. Chueh**

4:10 ENFL **316.** Hybrid (organic/inorganic) electrode design from bacterially precipitated CdS for PEC/storage applications. **Y. Feng**, E. Ngaboyamahina, K. Marusak, J.T. Glass, S. Zauscher

4:30 ENFL **317.** Impact of monolayer of alkyl amine on the crystalline orientation and performance of $CH_3NH_3PbI_3$ solar cells. **M. Ong**, Q. Liu, A. Lopez, X. Wang, D. Jiang, F. Zhou

4:50 Concluding Remarks.

Section D

Grand Hyatt San Francisco
Curran

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Energy Sources & Combustion

Cosponsored by ANYL

K. Herwig, R. E. Winans, *Organizers*

A. Ramirez-Cuesta, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **318.** Solvent swelling and surface energies in sequentially processed polymer:fullerene solar cells: Controlling vertical phase segregation in organic photovoltaics. **P. Yee**, M.T. Fontana, R. Huber, J.C. Aguirre, S.A. Jenekhe, B.J. Schwartz, S.H. Tolbert

2:05 ENFL **319.** *In-situ* SAXS studies of the density fluctuations of supercritical n-heptane. **S. Lee**, S. Lee, R.E. Winans

2:35 ENFL **320.** *In-situ* x-ray scattering and neutron imaging of combustion: Nanoparticles/soot and their formation and phase transitions. **F. Ossler**

3:05 Intermission.

3:20 ENFL **321.** New insights into thermal effect of crude oil adsorbed clay minerals by *in situ* USAXS/SAXS study. **S. Lee**, R.J. Klingler, J. Ilavsky, R.E. Winans, T. Fischer, D.K. McCarty, M.O. Wigand

3:50 ENFL **322.** Effect of surfactant adsorption on pore accessibility and water uptake in organic-rich shales. **S. Das**, J. Adeoye, B. Ellis

4:20 ENFL **323.** XRF analysis of water pretreated/leached banagrass to determine the effect of temperature, time and particle size on the removal of inorganic elements. **T.J. Morgan**, L.K. Andersen, H. Cui, S. Turn

4:50 Concluding Remarks.

Section E

Grand Hyatt San Francisco
Sequoia

Innovative Chemistry & Materials for Electrochemical Energy Storage

2D Energy Storage Materials

Cosponsored by MPPG‡ and PMSE

J. Guo, Y. Mo, *Organizers*

E. Pomerantseva, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **324.** 2D materials for energy storage and electrochemical actuation. **M. Chhowalla**

2:05 ENFL **325.** Few layered black phosphorus nanosheets for Li/Na storage. **A. Yan**

2:35 ENFL **326.** Two-dimensional transition metal carbides – New materials for electrochemical capacitors. **M. Lukatskaya**, Y. Gogotsi

3:05 Intermission.

3:15 ENFL **327.** Nanostructured bilayered V_2O_5 cathode for rechargeable batteries: Na- and Mg- ion case. S. Tepavcevic, Y. Liu, V. Stamenkovic, C.S. Johnson, **T. Rajh**

3:45 ENFL **328.** Design of materials for energy storage. **C.S. Ozkan**

4:15 ENFL **329.** Layered nanocomposites for energy storage. **N. Kotov**

4:45 ENFL **330.** High performance electrochemical capacitors based on conductive two-dimensional frameworks. **M. Lukatskaya**, D. Feng, T. Lei, Z. Bao

Section F

Grand Hyatt San Francisco
Cypress

Biomass & Biofuel Processing

Cosponsored by CELL, MPPG‡ and WCC

J. Fu, S. Turn, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **331.** Effect of feedstock and pyrolysis-catalyst on the yield of hydrotreated refinery intermediate. **R.J. French**, D. Carpenter, D. Howe, T.L. Westover

1:55 ENFL **332.** Pd nanoparticles stabilized in polymeric matrix in fatty acid hydrodeoxygenation. A. Stepacheva, V. Matveeva, J. Wärnå, P. Mäki-Arvela, D. Murzin, **E. Sulman**

2:15 ENFL **333.** Quantitative depolymerization of uncondensed technical lignin at 120 °C with supported nickel catalysts. **L. Shuai**

2:35 ENFL **334.** Deoxygenation of triglycerides in catalytic cracking process with enhanced hydrogen transfer activity. **I. Shimada**, S. Kato, N. Hirazawa, Y. Nakamura, H. Ohta, K. Suzuki, T. Takatsuka

2:55 Intermission.

3:10 ENFL **335.** Magnetically recoverable catalysts for cellulose conversion into ethylene- and propylene glycols. **E. Sulman**, O. Manaenkov, J.J. Mann, Y. Losovyj, B. Stein, O. Kislitza, D.G. Morgan, M. Pink, Z. Shifrina, V. Matveeva, L. Bronstein

3:30 ENFL **336.** Next-generation biomass fractionation with deep eutectic solvents. **M.B. Foston**, J. Meyer

3:50 ENFL **337.** Catalytic pulping of wood. R.C. Johnston, J.M. Parks, A. Rudie, J.J. Bozell, **T.J. Elder**

4:10 ENFL **338.** Co-extraction of hemicelluloses and polyphenolic compounds from four hardwood species using pressurized hot water: Influence of the process on extraction yields and mechanisms. **N. Beaufils**, L. Candy, P. Pontalier, L. Rigal, G. Vilarem

Catalytic Conversion of Lignocellulosic Biomass to Fuels, Chemicals & Materials

Sponsored by CATL, Cosponsored by CARB and ENFL

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Novel Photocatalytic & Photoelectrode Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

WEDNESDAY MORNING

Section A

Grand Hyatt San Francisco
Belvedere

Advances in Chemistry of Energy & Fuels

Fuel Life Cycle & Analysis

D. J. Heldebrant, *Organizer*

A. Padmaperuma, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **339.** Molecular characterization of Dissolved Organic Matter (DOM) in petroleum refinery wastewater by FT-ICR MS with ±ESI and +APPI ionization. **C. He**, Z. Fang, Y. Li, S. Zhao, Q. Shi

8:55 ENFL **340.** Impact of biodiesel blends on chemical composition of nitro-PAH and carbonyl compound emissions and stimulation of inflammatory responses in cells. **Y. Han**, J. Kasumba, N.K. Fukagawa, B. Holmen

9:15 ENFL **341.** Computational analysis of the combustion and atmospheric decomposition of the cis and trans isomers of hydroxyalkenylperoxy radicals. **S. Mondal**, A. Davis

9:35 ENFL **342.** Comprehensive analysis of molecular compositional changes of crude oils during biosouring. **J. Nowak**, P. Shrestha, R. Weber, J.D. Coates, A. Goldstein

9:55 Intermission.

10:00 ENFL **343.** Effects of thermal cracking of N-decane on ignition delay time in shock tube. **P. Shan-Shan**, G. Liu, X. Zhang, L. Wang, G. Li

10:20 ENFL **344.** Distribution, qualitative, and quantitative analyses of chlorides in distillates from ZJ crude oil. **R. Ma**, J. Zhu, B. Wu, X. Li, J. Xue

10:40 ENFL **345.** Hindered diffusion of sulfur-containing compounds in residue fractions through membranes and catalyst. **Z. Chen**, **K. Yuan**, M. Zheng, B. Wang, C. Xu

11:00 Concluding Remarks.

Section B

Grand Hyatt San Francisco
Filmore C

Functional Porous Materials for Sustainable Energy

Cosponsored by CATL and MPPG‡

R. Motkuri, N. L. Rosi, *Organizers*

S. Shanmugam, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **346.** New family of catalysts for solar fuels: Cofactor-like catalysts on mesoporous MOF supports. **J.T. Hupp**, O.K. Farha, A. Peters

9:00 ENFL **347.** Porosity gradient within metal-organic frameworks. **C. Liu**, N.L. Rosi

9:20 ENFL **348.** Surface modification of metal-organic framework nanoparticles through controlled radical polymerization: A general approach. **T. Li**, S. He

9:40 ENFL **349.** Porous and layered materials for gas sorption and separation applications. **E. Muthusamy**

10:00 Intermission.

10:10 ENFL **350.** Functional metal-organic frameworks for the energy-intensive separations. **M. Eddaoudi**, A. Cadiau, K. Adil, Y. Belmabkhout, P. Bhatt

10:30 ENFL **351.** Dehydrobenzoannulene-based covalent organic frameworks. **P. McGrier**

10:50 ENFL **352.** Reusable photocatalytic metal-organic frameworks for organic transformations. **X. Yu**, S. Cohen

11:10 ENFL **353.** Robust metal organic frameworks for adsorption chiller applications. **R. Vemuri**, J. Zheng, P. McGrail

11:30 Concluding Remarks.

Section C

Grand Hyatt San Francisco
Orpheum

13th International Symposium on Heavy Oil Upgrading, Production & Characterization

Cosponsored by CATL

C. Mesters, Y. Zhang, *Organizers*

J. J. Adams, *Organizer, Presiding*

Y. Zhang, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **354.** Basic research of solvent deasphalting coupling fluidization thermal conversion process for heavy oil. **H. Song**

8:55 ENFL **355.** Subsurface upgrading of heavy oils via solvent deasphalting. **C.F. Ovalles**

9:15 ENFL **356.** Effect of solvent and solvent-to-bitumen ratio on the liquefying point of asphaltenes in the solvent deasphalting process. **A. Turuga**, A. De Klerk

9:35 ENFL **357.** Nature of virgin and generated asphaltenes from thermal and/or steam catalytic cracking of Athabasca bitumen vacuum residue and its deasphalted oil. **L.A. Carbognani**, E. Rogel, C. Ovalles, F.A. Lopez-Linares, J. Carbognani, P. Pereira Almao, J. Vien, A. Pradhan

9:55 ENFL **358.** Propane-Steam Assisted Gravity Drainage (propane-SAGD) as a follow-up process to SAGD. T. Kar, C. Ovalles, I. Benson, **B. Hascakir**

10:15 Intermission.

10:30 ENFL **359.** 1350 F^+ by in-line filtration coupled with ICP-MS. **F.A. Lopez-Linares**, L. Poirier, C.F. Ovalles, E. Rogel, J. Nelson

10:50 ENFL **360.** Heat induced fouling of crude oils related to asphaltene stability and composition. **J.J. Adams**, P. Eaton, J.F. Schabron

11:10 ENFL **361.** Fouling apparatus to measure heat induced asphaltenic fouling of crude oils. **J.J. Adams**, R. Grimes, J.F. Schabron

Section D

Grand Hyatt San Francisco
Curran

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Fuel Cells

Cosponsored by ANYL

K. Herwig, R. E. Winans, *Organizers*

S. Lee, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **362.** Using neutron imaging to understand transport phenomenon in fuel cell and batteries. **D.L. Jacobson**, D. Hussey, J. LaManna, E.M. Baltic

9:05 ENFL **363.** Using small angle x-ray scattering as a key tool to develop next generation polymer electrolyte membrane for electrochemical energy conversion. **A.M. Herring**, A. Motz, Y. Liu, H. Sarode, T. Pandey

9:35 ENFL **364.** X-ray absoprtion spectroscopy characterization of bimetallic iron-nickel nanoparticle electrocatalysts. **L.F. Greenlee**, S. Candelaria

10:05 Intermission.

10:20 ENFL **365.** Revealing oxygen anion transport pathways in SOFC materials through in-situ neutron diffraction. **S. McIntosh**, A. Huq, A. Tomkiewicz, M. Tamimi, C. Sarno

10:50 ENFL **366.** Application of high resolution neutron imaging to polymer electrolyte fuel cells. **R. Mukundan**, D. Spernjak, D. Hussey, D.L. Jacobson, R. Borup

11:20 Concluding Remarks.

Section E

Grand Hyatt San Francisco
Sequoia

Innovative Chemistry & Materials for Electrochemical Energy Storage

Electrolytes & Interface

Cosponsored by MPPG‡ and PMSE

Y. Mo, E. Pomerantseva, *Organizers*

J. Guo, *Organizer, Presiding*

8:30 ENFL **367.** Anion-redox batteries and lithium metal protection. **J. Li**

9:00 ENFL **368.** Spontaneously formed interfacial phases for energy applications. **J. Luo**

9:30 ENFL **369.** Crosslinkable organic-inorganic hybrimer as binders for thermal stability-enhanced ceramic coated separator. **B. Jung**, S. Yang, H. Choi, B. Lee, M. Park, S. Han

9:50 ENFL **370.** Development of a highly conductive PEO-based solid polymer electrolyte. **C.C. Browder**

10:10 ENFL **371.** Stabilizing water in batteries. **K. Xu**

10:40 ENFL **372.** Computational study of the operation mechanism of tris(trimethylsilyl) phosphite as a multi-functional additive for lithium-ion batteries. **D. Kim**, H. Park, W.I. Choi, B. Roy, J. Seo, I. Park, Y. Kang, M. Koh

11:00 ENFL **373.** Interface identification of the solid electrolyte interphase on graphite. **E. Zvereva**, D. Caliste, P. Pochet, T. Deutsch

11:20 ENFL **374.** Substituent effects on the enhanced thermal stability of organosilicon electrolytes for lithium-ion batteries. **S.L. Guillot**, A. Peña-Hueso, M. Usrey, R.J. Hamers

11:40 ENFL **375.** Insights into the sodium-oxygen battery cathode electrochemistry. **J.E. Nichols**, B.D. McCloskey

12:00 ENFL **376.** High-loading sulfur-graphene oxide electrodes toward practical Li/S cells. Y. Hwa, **E.J. Cairns**

Section F

Grand Hyatt San Francisco
Cypress

Biomass & Biofuel Processing

Cosponsored by CELL, MPPG‡ and WCC

J. Fu, S. Turn, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **377.** Determination of bio-originated fuel content using a modified direct LSC method in the presence of quenching. **C. Doll**, C.W. Wright, S.M. Morley, B. Wright

8:55 ENFL **378.** Transportation fuels derived from biomass: Qualitative and quantitative analysis of reactive species. **A.B. Padmaperuma**, M.V. Olarte

9:15 ENFL **379.** Assessing factors responsible for lignocellulosic biomass saccharification: Fluorescence is brilliant. T. Auxenfans, B. Chabbert, **G. Paes**

9:35 ENFL **380.** Fluorescent probes dynamics to determine biomass characteristics impact on lignocellulolytic enzymes activity and mobility. **M. Herbaut**, G. Paes

9:55 Intermission.

10:10 ENFL **381.** Sustainable technologies towards a biorefinery: Extraction and tunable enrichment of microalgal triacylglyerides using supercritical carbon dioxide. **T.A. Kwan**, J.B. Zimmerman

10:30 ENFL **382.** Kinetics of phosphate precipitation from the nutrients-rich algal hydrolyzate. **A. Teymouri**, B. Stuart, S. Kumar

10:50 ENFL **383.** Maximizing atom (N, P, & C) economy via process integration in the conversion of microalgae to bioproducts and biofuels. A. Teymouri, C.R. Talbot, A. Samaratunga, B. Stuart, **S. Kumar**

11:10 ENFL **384.** Parametric optimization of syngas production from algal biomass gasification via central composite design. **A. Raheem**, R. Harun, M. Zhao

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Spectroscopy & Microscopy of Photocatalytic & PEC Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

‡ *Cooperative Cosponsorship*

WEDNESDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Belvedere

Advances in Chemistry of Energy & Fuels

Biomass & Biofuels

D. J. Heldebrant, *Organizer*

A. Padmaperuma, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **385.** Potential additives to improve biofuels properties and their effects on fuel characteristics. **J. Fu**, S. Turn

1:55 ENFL **386.** Lignin-derived multi-cyclic high density biofuel by alkylation and hydrogenated intramolecular cyclization. **G. Nie**, J. Zou, X. Zhang

2:15 ENFL **387.** Chemical reactions and structural identification of a coniferyl alcohol dimer causing instability in wood-derived pyrolysis oils. **J. Joseph**, M. Rasmussen, E.A. Stemmler, B. Jensen, B.G. Frederick

2:35 ENFL **388.** Preparation of bimetallic catalysts and activity test on hydrodeoxygenative upgrading of bio-oil. **S. Oh**, J. Choi

2:55 Intermission.

3:05 ENFL **389.** Tailor-made organic heterogeneous catalysts for the continuous-flow production of alkyl levulinates. **L. Vaccaro**, A. Marrocchi, V. Trombettoni

3:25 ENFL **390.** Sterically protected and electronically activated azamacrocycle catalysts for lignin depolymerization: A new approach to biomass valorization. **M. Chorghade**

3:45 ENFL **391.** Performance and structural evaluation of the torrefaction of bamboo under a high gravity (higee) environment using a rotating packed bed. M.G. de Luna, **M.V. Pillejera**, W. Chen

4:05 ENFL **392.** Development of novel nitrogenous base-tethered cobalt-Schiff base complexes for the selective catalytic cleavage of lignin. **R.E. Key**, J.J. Bozell

4:25 Concluding Remarks.

Section B

Grand Hyatt San Francisco
Filmore C

Functional Porous Materials for Sustainable Energy

Cosponsored by CATL and MPPG²

N. L. Rosi, S. Shanmugam, *Organizers*

R. Motkuri, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **393.** Porous metal-organic framework materials for gas storage and separation. **B. Chen**

1:55 ENFL **394.** Metal-organic framework templated low temperature CO oxidation catalysts. **C.W. Abney**, J.T. Patterson, G. Veith, R. Unocic, S. Dai

2:10 ENFL **395.** Synthesis of benzobisoxazole-linked two-dimensional covalent organic frameworks & their properties for carbon-dioxide capture. **D. Pyles**, J. Crowe, L. Baldwin, P. McGrier

2:25 ENFL **396.** Microporous graphene-like frameworks for gas and energy storage applications. **A. Coskun**

2:40 Intermission.

2:50 ENFL **397.** Advanced porous organic polymers: Task-specific design and functionalization. **S. Ma**

3:10 ENFL **398.** Hierarchical porous carbon materials platform with exceptional surface area and pore volume for energy and environmental applications. **L. Estevez**, J. Zheng, A. Garcia, R. Vemuri, S. Jeong, W. Xu, P. Bhattacharya, X. Li, Y. Shin, R. Motkuri, J. Zhang

3:25 ENFL **399.** Microporous materials for the effective adsorption and separation of CO_2 from flue gases. **S. Prodinger**, M.A. Derewinski, R. Motkuri

3:40 Concluding Remarks.

Section C

Grand Hyatt San Francisco
Orpheum

13th International Symposium on Heavy Oil Upgrading, Production & Characterization

Cosponsored by CATL

C. Mesters, Y. Zhang, *Organizers*

J. J. Adams, *Organizer, Presiding*

Y. Zhang, *Presiding*

1:30 ENFL **400.** Monitoring production and transportation of heavy crude oil using near infrared spectroscopy. **T. Miao**, A.R. Pradhan, M. Moir, E. Lee

1:50 ENFL **401.** Comparisons and structural characterization of petroleum cut samples from different origins: Impact of hydrotreatment processes. F. Albrieux, J. Barbier, **J. Ponthus**

2:10 ENFL **402.** Molecular composition building strategies for petroleum feedstock. **S. He**, L. Zhang, Q. Shi, S. Zhao

2:30 ENFL **403.** Molecular characterization of sulfur-containing compounds in vacuum residue by FT-ICR MS and GC×GC-TOFMS. **X. Cai**, W. Wang, J. Zhou, Z. Liu, Y. Liu, S. Tian

2:50 ENFL **404.** Characterization and behavior of interfacially active asphaltenes from crude oil. **J.J. Adams**, J.F. Schabron, J. Loveridge, R. Grimes, L. Goual, G. Javanbakht

3:10 ENFL **405.** Molecular-level analysis of petroleum interfacially active species reveals the components responsible for stable emulsion formation. **R.P. Rodgers**, Y. Corilo, D.C. Podgorski, S. Rowland, P.M. Lalli, W.K. Robbins, A.C. Clingenpeel

3:30 Intermission.

3:45 ENFL **406.** Study of asphaltene retention on iron oxide under poor solvent conditions. **E. Rogel**, M. Roye

4:05 ENFL **407.** Influence of metal halides on coke formation. **G. Carvalho do Prado**, Riya, M. Hyrve, A. De Klerk

4:25 ENFL **408.** Reservoir rock-asphaltenes interaction impacts asphaltenes stability. **B. Hascakir**

Section D

Grand Hyatt San Francisco
Curran

Applications of X-Ray & Neutron Scattering Techniques in Energy Technologies

Gas Storage & Ion Conduction

Cosponsored by ANYL

R. E. Winans, *Organizer*

K. Herwig, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **409.** Characterizing phase transitions in metal-organic frameworks and nanoparticle superlattices. **J.A. Mason**, J.R. Long, C.A. Mirkin

2:05 ENFL **410.** Neutron scattering studies of hydrogenous materials for next-generation energy storage. **M. Dimitrievska**, W. Tang, H. Wu, W. Zhou, T.J. Udovic

2:35 ENFL **411.** Functional porous materials for guest storage, selectivity and catalysis. **S. Yang**

3:05 Intermission.

3:20 ENFL **412.** Neutron scattering to probe battery interfaces and dynamics. **G. Veith**, J. Browning, M. Doucet, J. Kim

3:50 ENFL **413.** Neutron scattering studies on atomic-scale proton diffusion processes in a solid oxide electrolyte. **N. Jalarvo**, Y. Cheng, J. Balachandran, P. Ganesh, C.A. Bridges, M. Paranthaman, Z. Bi, D. Gout, O. Gourdon

4:20 Concluding Remarks.

Section E

Grand Hyatt San Francisco
Sequoia

Innovative Chemistry & Materials for Electrochemical Energy Storage

Anode Materials & Li-S

Cosponsored by MPPG² and PMSE

Y. Mo, E. Pomerantseva, *Organizers*

J. Guo, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENFL **414.** Design principles of non-graphitic carbon electrodes for energy storage. Z. Li, Z. Jian, C. Bommier, P. Greaney, **X. Ji**

2:05 ENFL **415.** Enhanced performance of high volumetric energy density sulfur cathode for Li-sulfur batteries. **D. Lv**, J. Liu, Q. Li, S. Chen, G. Graff, J. Zhang, J. Liu

2:35 ENFL **416.** Boron doped fullerene based materials for electrochemical applications. **P. Sood**, K. Kim, S.S. Jang

2:55 ENFL **417.** Electrospinning-assisted and self-assembled construction of hybrid SnO_2-Co_3O_4 nanotubes for greater lithium storage properties. **J. Zhang**

3:15 ENFL **418.** High-performance Ge microwire Li-ion battery anodes as prepared by the electrochemical liquid-liquid-solid deposition process at T = 80 °C. **L. Ma**, E. Fahrenkrug, E. Gerber, A. Crowe, F.A. Venable, B.M. Bartlett, S. Maldonado

3:35 Intermission.

3:45 ENFL **419.** Discrete nanographene encapsulated Si nanoparticles and their properties as Li-ion battery anode. **B. Li**, **D. Zhao**, C. Niu

4:05 ENFL **420.** Rational design of silicon nanolayer embedded macroporous carbon micro-cages for high energy and power lithium-ion batteries. **Y. Son**, J. Ma, J. Cho

4:25 ENFL **421.** Overcoming micro-silicon particle fracture within graphene cages for stable battery anodes. **Y. Li**, Y. Cui

4:45 ENFL **422.** Edge plane-activated graphite/Si composite for lithium ion battery anodes: Toward fast charge capabilities at high energy density electrodes. J. Cho, **N. Kim**

5:05 ENFL **423.** Low-cost tire-derived carbon/metal oxide composite electrodes for improved high-capacity lithium-ion battery anodes. **Y. Li**, A.M. Levine, R. Lee, K. Akato, A.K. Naskar, S. Dai, M. Paranthaman

Section F

Grand Hyatt San Francisco
Cypress

Biomass & Biofuel Processing

Cosponsored by CELL, MPPG² and WCC

J. Fu, S. Turn, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 ENFL **424.** Operational issues using biomass-derived feedstocks in a Davison circulating riser. **J. Olstad**, M. Jarvis, Y. Parent, K.A. Magrini

1:55 ENFL **425.** Potential applications of alkali metal sorbents (Li_2ZrO_3, Li_4SiO_4 and Na_2ZrO_3) as bifunctional material for biomass gasification. **M.H. Memon**, M. Zhao

2:15 ENFL **426.** Novel alkaline thermal treatment of biomass for hydrogen production with carbon capture and storage potential. **A.A. Park**, M. Stonor, J.G. Chen

2:35 ENFL **427.** Reversibility of the reaction catalyzed by the molybdenum-containing formate dehydrogenase from *Cupriavidus necator* (*Ralstonia eutropha*). **X. Yu**, D. Niks, R. Hille, A.K. Mulchandani

2:55 Intermission.

3:10 ENFL **428.** Role of materials derived from biodiesel production on cold flow properties of model biodiesel. **M. Senra**, L. Soh, R. Elias, S. McCartney

3:30 ENFL **429.** Homogeneous catalytic biodiesel production from wet spent coffee grounds by integrating lipid extraction and conversion. **J. Park**, B. Kim, J.W. Lee

3:50 ENFL **430.** Combined production of levulinic acid and sulfonated carbon from glucose in one-pot reaction. **S. Kang**, **G. Zhang**, **F. Qin**, **X. Fu**, **H. Yin**, **Y. Xu**

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Devices, Assemblies & Hybrid Processes

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

THURSDAY MORNING

Section A

Grand Hyatt San Francisco
Belvedere

Advances in Chemistry of Energy & Fuels

Fuels & Lubricants

D. J. Heldebrant, *Organizer*

A. Padmaperuma, *Presiding*

8:30 Introductory Remarks.

8:35 ENFL **431.** Composition-property relationships of hydrocarbon fuels based on GC×GC–MS/FID. **X. Shi**, **G. Liu**, **X. Zhang**, **L. Wang**, **G. Li**

8:55 ENFL **432.** Characterization of petroleum using borate fusion and ICP-OES analyses. **J. Anzelmo**, P. Daigle, J. Pitre

9:15 ENFL **433.** Correlating crude oil and kerogen properties to asphaltene fractions using infrared spectroscopy and chemometrics. **R.F. Dias**, J.E. Birdwell

9:35 ENFL **434.** Contribution to the total acid number of petroleum phenols and its response in electrospray mass spectrometry analysis. **M. Hu**, C. Xu, Q. Shi

9:55 ENFL **435.** Molecular composition analysis of lubricant base oils by using RICO redox derivatization followed by ESI FT-ICR MS. **S. Ma**, C.S. Hsu, Y. Zhou, Q. Shi

10:15 Intermission.

10:25 ENFL **436.** Computer-aid gasoline molecular composition reconstruction on the basis of GC-FID data. **C. Cui**, L. Zhang, Q. Shi, S. Zhao

10:45 ENFL **437.** Multiobjective feature selection approach to Quantitative Structure Property Relationship (QSPR) for predicting the octane number of compounds found in gasoline. **Z. Liu**, L. Zhang, A. Elkamel, S. Zhao, C. Xu

11:05 ENFL **438.** Developing a high- and low-cetane classifier for biologically produced chemicals using variable quality training data. L.S. Whitmore, R.L. McCormick, R.W. Davis, J.M. Gladden, B.A. Simmons, A. George, **C. Hudson**

11:25 ENFL **439.** Aluminum nanoparticles as energy additive of jet fuel: Synthesis, stability, ignition, and propulsion performance. **X. E**, J. Zou, X. Zhang

11:45 ENFL **440.** Understanding and characterization of 100 low lead aviation fuels for general aviation. **C. Huang**

12:05 Concluding Remarks.

Section B

Grand Hyatt San Francisco
Union Square

Functional Porous Materials for Sustainable Energy

Cosponsored by CATL and MPPG‡

R. Motkuri, S. Shanmugam, *Organizers*

N. L. Rosi, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **441.** Linker engineering on metal-organic frameworks as a platform for sustainable catalysis. **W. Huang**, L.M. Stanley, X. Li, R. Van Zeeland

8:55 ENFL **442.** Investigating bulk-like vapor-liquid coexistence in microporous metal-organic frameworks via molecular simulations and NMR relaxometry. **E. Braun**, S.K. Schnell, J.A. Reimer, B. Smit

9:10 ENFL **443.** Withdrawn.

9:25 ENFL **444.** Adsorptive desulfurization over mesoporous materials. **G. Liu**, Y. Shi, X. Zhang

9:40 Intermission.

9:50 ENFL **445.** Porous metal-organic frameworks for Li–O_2 and Li–ion batteries. Y. Wang, Y. Zhao, **Q. Li**

10:05 ENFL **446.** Synthesizing particulate carbon with controlled morphology. **H. Ho**, A.K. Naskar

10:20 ENFL **447.** Cobalt-containing Porous Organic Polymer (POP) as precursor of new electrode catalyst for oxygen reduction reaction. **Y. Yuan**, D. Liu

10:35 ENFL **448.** Synthesis and characterization of SBA-15 supported catalysts for styrene oxidation. **S. Sharma**, V. Chaudhary

10:50 Concluding Remarks.

Section C

Grand Hyatt San Francisco
Sunset

13th International Symposium on Heavy Oil Upgrading, Production & Characterization

Cosponsored by CATL

C. Mesters, Y. Zhang, *Organizers*

J. J. Adams, *Organizer, Presiding*

Y. Zhang, *Presiding*

8:30 ENFL **449.** Detailed characterization of vacuum residue through hydrotreatment and hydrocracking for marine fuel application. **W. Weiss**, I. Merdrignac, J. Barbier

8:50 ENFL **450.** Study on the FCC process in a downer reactor. **C. Zhang**, W. Qian, F. Wei

9:10 ENFL **451.** Development of functionalized polymers for the removal of nitrogen and sulfur compounds from bitumen-derived heavy gas oil. **P. Misra**, S. Badoga, A. Dalai, J. Adjaye

9:30 ENFL **452.** Customized catalyst for MIP process to increase cleaner gasoline and propylene production. **J. Gong**, W. Jiang

9:50 ENFL **453.** Acceleration of TiO_2-catalyzed oil upgrading in microdroplets. **Y. Lai**, Z. Zhou, C. Basheer, R. Zare

10:10 Intermission.

10:25 ENFL **454.** High-resolution mapping of core and shale samples: Combination of laser-induced breakdown spectroscopy with infrared microscopy for advanced characterization. **F.A. Lopez-Linares**, D. Quarles, J. Gonzalez, T. Miao, L. Poirier

10:45 ENFL **455.** Carbon dioxide storage in heavy oil reservoirs. **B. Hascakir**

11:05 Concluding Remarks.

Section D

Grand Hyatt San Francisco
Curran

Innovative Chemistry & Materials for Electrochemical Energy Storage

Electrochemical Catalysis & Energy Conversion

Cosponsored by MPPG‡ and PMSE

Y. Mo, E. Pomerantseva, *Organizers*

J. Guo, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENFL **456.** Construction and intelligent manipulation of nanocarbon composite electrodes toward energy storage and mechanical conversion devices. **G. Wu**

8:55 ENFL **457.** Solar-driven water oxidation and decoupled hydrogen production mediated by an electron-coupled-proton buffer. **L. Cronin**

9:15 ENFL **458.** Facile synthesis of 3D PtBi intermetallic nanoplates with highly catalytic activity toward methanol/ethanol oxidization. **X. Yuan**, Q. Zhang

9:35 ENFL **459.** Series of ionomers and their SiO_2-TiO_2 inorganic-organic nanocomposites for PEM fuel cells. **F. Huang**, T.D. Largier, B. Motealleh, C.J. Cornelius

9:55 Intermission.

10:05 ENFL **460.** Synthesis and characterisation of Au-Ru core-branched nanoparticles for oxygen evolution reaction catalysts. **L. Gloag**, S. Cheong, Y. Li, C. Zhao, J. Gooding, R. Tilley

10:25 ENFL **461.** Valence- and element-dependent water oxidation behaviors: *In-situ* x-ray scattering, absorption and electrochemical impedance spectroscopies. **H. Chen**

10:45 ENFL **462.** Sulfonated poly(phenelyne)s/novel branched polysulfone-based polymer blend for PEM fuel cell. **B. Motealleh**, T.D. Largier, F. Huang, C.J. Cornelius

11:05 ENFL **463.** High-performance flexible thermoelectric generator based on carbon nanotube yarn. **J. Choi**, Y. Jung, H. Kim, C. Park

‡*Cooperative Cosponsorship*

ENVR

Division of Environmental Chemistry

S. Obare and S. Al-Abed, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

ACS-CEI Award for Incorporating Sustainability into Chemistry Education (see *CHED*, Mon)

Perspectives on Climate Change Literacy & Education: Local to International (see *CHED*, Tue)

Environmental Challenges & Solutions in Unconventional Oil & Gas Development (see *GEOC*, Wed, Thu)

Elucidation of Mechanisms & Kinetics on Surfaces (see *CATL*, Sun, Mon, Tue, Wed, Thu)

Mineral-Water Interface Chemistry: A Tribute to Glenn Waychunas (see *GEOC*, Sun, Mon, Tue, Wed)

Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy (see *CELL*, Mon)

SOCIAL EVENTS:

Reception, 6:00 PM: Tue

Breakfast, 7:45 AM: Mon

BUSINESS MEETINGS:

Program Planning Committee Meeting, 2:00 PM: Sun

Long Range Planning Committee Meeting, 3:00 PM: Sun

Executive Committee Meeting, 7:00 PM: Sun

SUNDAY MORNING

Section A

San Francisco Marriott Marquis
Salons 10/11

Tribute to Jerry Schnoor

J. G. Burken, D. M. Cwiertny, C. L. Just, *Organizers*, *Presiding*

8:30 ENVR **1.** Climate change adaptation for infrastructure: A grand challenge for civil and environmental engineering. **D.A. Dzombak**, C. Samaras

9:00 ENVR **2.** Mechanisms governing algal mitigation of atmospheric CO_2 in shallow saline lakes of the Chilean Altiplano region. **A.L. Prieto**, A. de la Fuente

9:20 ENVR **3.** Substrate specificity of kinetic isotope effects associated with the dioxygenation of (nitro)aromatic contaminants is due to uncoupling of O_2 activation. **S.G. Pati**, H.E. Kohler, A. Pabis, P. Paneth, R.E. Parales, T.B. Hofstetter

9:40 ENVR **4.** Carbon and nitrogen isotope fractionation reveals the biodegradation of 2,4-dinitroanisole. **T.B. Hofstetter**, J. Bolotin, M. Palatucci, J.C. Spain

10:00 Intermission.

10:15 ENVR **5.** From phytoremediation to nanotechnology: A tribute to Jerald Schnoor. **J.L. Gardea-Torresdey**

10:45 ENVR **6.** Nanoparticle surface affinity as a predictor of trophic transfer. **N. Geitner**, S. Marinakos, C. Guo, N. O'Brien, M. Wiesner

11:05 ENVR **7.** Impact of cerium oxide nanoparticles on the uptake and accumulation of cadmium in soybean (*Glycine max L.*). **X. Ma**, L. Rossi, P. Schwab

Section B

San Francisco Marriott Marquis

Salons 12/13

Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in honor of Prof. Jun Ma

Oxidation Processes

Financially supported by Sciex China

D. D. Dionysiou, J. Fang, *Organizers*

V. K. Sharma, *Organizer, Presiding*

A. T. Stone, *Presiding*

8:30 Introductory Remarks.

8:40 ENVR **8.** Bi_2WO_6-graphene nanocomposites with laminar structure for environmental remediation. B. Ren, M. Nadagouda, **D.D. Dionysiou**

9:05 ENVR **9.** Photocatalytic inactivation mechanisms of bacteria as well as the decomposition of Antibiotic-Resistance Genes (ARG). **G. Li**, H. Yin, Q. Jiang, **T. An**

9:30 ENVR **10.** Activation of peroxides by phosphate ion for water purification. **Y. Yang**, J. Kim, J.J. Pignatello

9:50 ENVR **11.** Degradation of the typical macrolide antibiotic roxithromycin by UV/H_2O_2: Reaction kinetics and degradation byproducts. **W. Li**, X. Xu, Y. Tang, Y. Zhang

10:10 Intermission.

10:25 ENVR **12.** Overlooked oxidation states of chemical elements in treatment plants and the environment: Interconnections between speciation and reactivity. **A.T. Stone**, X. Xia, W. Liao

10:50 ENVR **13.** Catalytic ozonation processes not relying on hydroxyl radical oxidation. **T. Zhang**

11:15 ENVR **14.** Role of the propagation reactions on the hydroxyl radical formation in the ozonation and catalytic ozonation of real waters. **Y. Liu**, J. Ma, J. Jiang, L. Zhang

11:35 ENVR **15.** Reaction kinetics and degradation pathway of antipyrine during chlorine dioxide disinfection process. **X. Jia**, L. Zhang, L. Feng, Y. Liu

Section C

San Francisco Marriott Marquis

Salons 14/15

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Cosponsored by CHED

Financially supported by AEESP

M. J. McGuire, F. L. Rosario, *Organizers*

J. A. Pedersen, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ENVR **16.** Three decades of research at CIRSEE Suez on taste and odor in drinking water, under the umbrella of Prof. I.H. Mel Suffet. **A.L. Bruchet**

8:35 ENVR **17.** Estimates of threshold, recognition and objection concentrations for crude 4-methylcyclohexanol and methyl t-butyl ether in water. **M.J. McGuire**, I.H. Suffet

9:00 ENVR **18.** Chemical spill of crude MCHM into the Elk River. **J. Rosen**

9:25 ENVR **19.** From Philly to smell A - tracking, measuring, and controlling non-H2S odor nuisances. **J. Witherspoon**, S. Cowden, I.H. Suffet

9:50 ENVR **20.** Importance of sensory analysis and odor activity values in the determination of odorants causing nuisance in the wastewater treatment process. **T. Vitko**, Y. Zhou, I.H. Suffet

10:15 Intermission.

10:30 ENVR **21.** Determination of the primary odor nuisances from wastewater treatment plants. Y. Zhou, T. Vitko, **I.H. Suffet**

10:55 ENVR **22.** Occurrence and fate of sensory compounds in water reuse. **S.W. Krasner**, A. Jia, C. Lee, T.R. Slifko

11:20 ENVR **23.** Two phase interactions: A lynchpin of environmental chemistry. **I.H. Suffet**

Section D

San Francisco Marriott Marquis

Golden Gate C1

Understanding Dissolved Organic Matter Reactivity: Honoring George Aiken, the DOM Whisperer

Y. Chin, *Organizer*

D. M. McKnight, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ENVR **24.** In defense of DOM molecular models. **J. Leenheer**

8:45 ENVR **25.** Investigation of the effect of solvent polarity and temperature on the optical properties of dissolved organic matter. **J.A. Korak**, G. McKay, P.R. Erickson, D.E. Latch, K.P. McNeill, G. Aiken, F.L. Rosario

9:10 ENVR **26.** Carbon tracing: Environmental applications of wet oxidation total organic carbon cavity ring-down spectroscopy. **C. Conaway**

9:35 ENVR **27.** High resolution mass spectrometry of leachate from soils subject to simulated wildfire heating. **J. Webster**, R. Young, T. Borch, F.L. Rosario

10:00 Intermission.

10:10 ENVR **28.** Using the reverse osmosis/electrodialysis method to isolate natural organic matter from rivers and estuaries in coastal Georgia. **E.M. Perdue**, S. Driver

10:45 ENVR **29.** Isolation of Dissolved Organic Matter (DOM) with XAD resins: Early studies. **E.M. Thurman**

11:10 ENVR **30.** Classification analysis of humic substances fractionated using size exclusion chromatography based on numerical descriptors generated from the data of Fourier transform mass spectrometry. **I.V. Perminova**, A.V. Kudryavtsev, M. Kazachkov, A. Konstantinov, E. Belyaeva, A. Gaspar, P. Schmitt-Kopplin, G. Abbt-Braun, F. Frimmel

11:35 ENVR **31.** Dependence of reduced sulfur in Everglades dissolved organic matter on sulfate enrichment. **B. Poulin**, J.N. Ryan, K.L. Nagy, T. Dittmar, A. Stubbins, W. Orem, D.P. Krabbenhoft, G. Aiken

Section E

San Francisco Marriott Marquis

Sierra A

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

D. D. Dionysiou, X. He, K. E. O'Shea, X. Quan, *Organizers*

G. Li Puma, D. Minakata, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **32.** Molecular modeling of aqueous radical chemistry: Estimating chemical properties and elucidating reaction pathways. **J. Arey**, P. Tentscher, J.J. Guerard, D. Trogolo

8:40 ENVR **33.** Linking treatment to toxicology – Screening for toxic transformation products formed during oxidative treatment of organic contaminants. **C. Prasse**, B. Drew-Ford, D. Nomura, D.L. Sedlak

9:05 ENVR **34.** Effect of solution conditions on reactive oxidant production during chlorine photolysis. **D. Manley**, C.K. Remucal

9:30 ENVR **35.** Enhancing photocatalytic degradation of the cyanotoxins microcystin-LR and nodularin with the addition of sulfate-radical producing oxidants. **M.G. Antoniou**, I. Boraei, D.K. Pantelide, M. Abhishek, C. Edwards, L. Lawton

9:55 Intermission.

10:10 ENVR **36.** Mechanistic insight into reactivity of chlorinated radicals in UV/chlorine advanced oxidation system. **D. Minakata**, D. Kamath, S. Maetzold, D. Perram

10:45 ENVR **37.** Ag/AgCl @ chiral TiO_2 nanofibers plasmonic photocatalyst for removal of contaminants of emerging concern in simulated and urban wastewater. **G. Li Puma**, D. Wang, Y. Li

11:10 ENVR **38.** Impact of halides on the degradation of amino acid residues in biomolecules. **Y. Komaki**, J. Choe, W. Mitch

11:35 ENVR **39.** Investigation of radical chloramine reaction kinetics and thermodynamics under advanced oxidation processes. **J. Gleason**, S.P. Mezyk, K.P. Ishida

Section F

San Francisco Marriott Marquis

Sierra B

Contaminants of Emerging Concern in Natural & Engineered Systems

Cosponsored by AGRO, ANYL and CEI

L. M. Blaney, A. J. Hernandez, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ENVR **40.** Mineral-catalyzed hydrolysis of organophosphorus flame retardants – a potential major fate-controlling sink in soil and aquatic environments. **Y. Fang**, E. Kim, T.J. Strathmann

8:55 ENVR **41.** Drug co-binding at mineral surfaces. **J. Xu**, R. Marsac, D. Costa, J. Boily, F. Wu, K. Hanna

9:15 ENVR **42.** Discrete molecular dynamics to screen for co-contaminant risk potential of nanomaterials in agriculture. **N. Geitner**, M. Wiesner

9:35 ENVR **43.** Molecular dynamics simulation and experimental study of the adsorption of phthalate esters on clay surfaces. **J. Willemsen**, I.C. Bourg

9:55 Intermission.

10:15 ENVR **44.** Fixed-bed adsorption of contaminants of emerging concern from water using Cu^{2+} amino grafted SBA-15. **K. Ortiz-Martinez**, F. Roman, A.J. Hernandez

10:35 ENVR **45.** Development of pH-responsive block copolymers membranes reinforced with nanocellulose for the adsorption of emerging contaminants. **J. Herrera**, L. Rivera, E.O. Ortiz Quiles, E. Nicolau

10:55 ENVR **46.** Withdrawn.

11:15 ENVR **47.** Withdrawn.

11:35 ENVR **48.** Simultaneous removal of multiple contaminants of emerging concern via biofiltration. **K. Greenstein**, J. Lew, E. Dickenson, E. Wert

11:55 Concluding Remarks.

Section G

San Francisco Marriott Marquis

Sierra C

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Cosponsored by ANYL

T. Anumol, R. Marfil-Vega, T. M. Young, *Organizers*, *Presiding*

8:00 ENVR **49.** Identification of known, suspected, and unknown contaminants by nontarget analysis of Polar Organic Chemical Integrating Sampler (POCIS) extracts. **E.T. Furlong**, L.K. Kanagy, W.T. Foreman, D.A. Alvarez

8:25 ENVR **50.** Broad-scope screening for organic contaminants in wastewater at the sub-sewershed scale to identify source contributions. **J. Teerlink**, C. Alaimo, T.M. Young

8:50 ENVR **51.** Organic contaminants monitoring during water treatments by UHPLC-HRAM: From influent to effluents. **D.D. Yang**, T. Anumol

9:15 ENVR **52.** When does a GAC filter become a biofilter for removing seasonal trace organics? Application of LC/QTOF analysis to evaluate (bio-) filter performance. **R. Marfil-Vega**, M. Surmeier, O. Schneider, E. Dickenson

9:40 ENVR **53.** Non-targeted analysis reveals a novel bacterial metabolite of pyrene implicated in genotoxicity of bioremediated soil. **Z. Tian**, A. Gold, J. Nakamura, Z. Zhang, J. Vila, D. Singleton, L. Collins, M. Aitken

10:05 Intermission.

10:20 ENVR **54.** LC/Q-TOF-MS for the identification of environmental metabolites and degradation products. **I. Ferrer**, E.M. Thurman, J. Zweigenbaum

10:45 ENVR **55.** Identifying Poly- and Perfluoroalkyl Substances (PFAS) transformation products in a wastewater treatment plant. E. Houtz, **M. Wang**, W. Duong, J. Park

11:10 ENVR **56.** Quantitative comparison of perfluorinated organic compounds in drinking water between tandem triple quadrupole MS/MS and high resolution mass spectrometry using orbitrap technology-knowns and unknowns. **E. George**

11:35 ENVR **57.** Comprehensive targeted and untargeted analysis of Per- and Polyfluoroalkyl Substances (PFASs) in Australian Wastewater and recycled water. **T. Coggan**, T. Anumol, B. Clarke

Section H

San Francisco Marriott Marquis

Sierra J

Green Chemistry & the Environment

Cosponsored by CEI

Financially supported by AEESP

A. M. Balu, R. Luque, *Organizers*

S. O. Obare, *Organizer, Presiding*

T. Dittrich, D. Vardon, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **58.** Orientation of organic synthesis in water. **C. Len**

8:40 ENVR **59.** Purification of environmental contaminants from post combustion carbon capture solvents. **S. Bhatnagar**, J. Thompson, F. Onneweer, M. Combs, K. Abad, H. Nikolic, K. Liu

9:00 ENVR **60.** Bio-based γ-valerolactone and furfuryl alcohol as novel reaction media. L. Vaccaro, **S. Santoro**

9:20 ENVR **61.** Bimetallic Ru-Sn/AC for the aqueous phase catalytic conversion of microbial acids to alcohols. **D. Vardon**, A. Settle, T. Eaton, V. Vorotnikov, G. Beckham

9:40 Intermission.

9:55 ENVR **62.** Measurement of heterocyclic aromatic amines as tracers of anthropogenic contributions to fine particulate matter. **D. Thai**, J. Miller-Schulze, A. Lai, M.R. Olson, J.J. Schauer

10:15 ENVR **63.** Microwave-induced target orientd synthesis of curcumin-pyrazole derivatives: Potentially important for neuroprotective properties in Alzheimer's disease. **B. Dayal**, B. Patel

10:35 ENVR **64.** Inorganic-organic microcapsule emulsion for surface and air disinfections. **W. Han**, Y. Lai, Q. Chang, H. Leung, Y. Li, Y. Yang, C. Wu, K. Yeung, J. Kwan, C. Chao, Z. Yang

10:55 ENVR **65.** Fe-assisted hydrothermal liquefaction of oil palm empty fruit bunch to bio-oil. **Y. Miyata**, K. Sagata, M. Hirose, Y. Yamazaki, A. Nishimura, N. Okuda, Y. Arita, Y. Hirano, Y. Kita

11:15 ENVR **66.** Kinetic study on the adsorption of humic acid fractions onto clay minerals. **M. ElSayed**, M. Khalaf, J. Rice

11:35 ENVR **67.** Formation of metal-humate complexes in sediments and environmental impact of heavy metal adsorption in the presence of humic acids. **J. Hizal Yücesoy**, R. Apak

Section I

San Francisco Marriott Marquis

Sierra K

Have Great Lakes Restoration Programs Been Successful? The Case of Legacy & Emerging Pollutants

J. J. Pagano, *Organizer*

K. C. Hornbuckle, *Organizer, Presiding*

8:00 ENVR **68.** Trends of legacy and emerging contaminants in the Great Lakes based on passive sampling of air and water. **R. Lohmann**, C. McDonough, Y. Liu, M. Khairy, P.A. Helm, D.C. Muir

8:30 ENVR **69.** Organophosphate flame retardants in the lower Great Lakes: Spatial distribution and air-water exchange. **C.A. McDonough**, P.A. Helm, D. Muir, R. Lohmann

8:50 ENVR **70.** Spatial and temporal trends of particle phase organophosphate ester concentrations in the atmosphere of the Great Lakes. **A. Salamova**, A. Peverly, M. Venier, R.A. Hites

9:10 ENVR **71.** Pharmaceuticals and personal care product chemicals in waters and fish in a Great Lakes urban wetland. **D.C. Muir**, X. Wang, D. Simmons, J. Sherry

9:30 ENVR **72.** GLFMSP Legacy and emerging chemical trends. B.S. Crimmins, **S. Fernando**, C. Zhou, H. Zhou, S. Fakouri Baygi, B. Parvizian, P.K. Hopke, T. Holsen, J.J. Pagano, M. Milligan

9:50 Intermission.

10:00 ENVR **73.** How do we reduce chemicals of concern in the Great Lakes after picking the low hanging fruit? **M.L. Diamond**, P.A. Helm, L. Jantunen, D. McGoldrick, J. Truong, A. Soehl

10:20 ENVR **74.** Concentration trends and elimination rates for polychlorinated dioxins/furans, and dioxin-like polychlorinated biphenyls in Lake Ontario salmonid eggs: 2004-2015. **A.J. Garner**, J.J. Pagano

10:40 ENVR **75.** Airborne PCBs and OH-PCBs inside and outside rural schools and urban schools near Lake Michigan. R.F. Marek, A. Awad, N. Herkert, P.S. Thorne, **K.C. Hornbuckle**

11:00 ENVR **76.** Impact of waves on contaminant fate in Great Lakes beach environments. **D.M. O'Carroll**, C. Robinson, S. Malott

11:20 ENVR **77.** Biomonitoring legacy and emerging Great Lakes contaminants in susceptible Great Lakes populations. **Z. Li**, W. Wattigney, S. Naik, E. Irvin-Barnwell, A. Ragin-Wilson

11:40 ENVR **78.** GLRI success: Educating government and business towards reducing PBDEs and other chemicals of concern in the Great Lakes and beyond. **A. Blum**, M.L. Diamond, G. Peaslee, A. Soehl

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Sponsored by GEOC, Cosponsored by COLL and ENVR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Elucidation of Mechanisms & Kinetics on Surfaces

Theory

Sponsored by CATL, Cosponsored by COLL and ENVR

SUNDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Salons 10/11

Tribute to Jerry Schnoor

J. G. Burken, D. M. Cwiertny, C. L. Just, *Organizers*, *Presiding*

1:30 ENVR **79.** My academic journey with electron transfer on Fe minerals and my U. Iowa colleague, Jerry Schnoor. **M. Scherer**, L.N. Andrade, Z. Zhou, J.D. Culpepper, D. Latta

2:00 ENVR **80.** Modeling adsorption of copper on goethite in natural water systems: Effect of solution chemistry. J. Han, S.M. Nomaan, **L.E. Katz**

2:20 ENVR **81.** Adsorption, aggregation, and morphological transformation of graphene and graphene oxide with binding pollutants in water. **B. Chen**, K. Yang, W. Jun, X. Zhu

2:40 ENVR **82.** Advancing materials and reactor design for catalytic technologies for treatment of nitrate-contaminated water. **T.J. Strathmann**, C.J. Werth, A. Bergquist, X. Huo

3:00 Intermission.

3:15 ENVR **83.** Environmental applications of nanoparticle-enabled sensing. **P.J. Vikesland**, H. Wei, W. Leng, V.R. Breazeal, M. Willner

3:45 ENVR **84.** Formation and properties of iron(III)-precipitates and their effects on the distribution and fate of phosphorous and arsenic in rice fields and in water treatment. **S.J. Hug**, A.C. Senn, R. Kaegi, A. Voegelin

4:05 ENVR **85.** Comparison of trace compound migration through a natural aquifer sand. **P. Behra**

Section B

San Francisco Marriott Marquis

Salons 12/13

Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in honor of Prof. Jun Ma

Iron & Manganese Chemistry

Financially supported by Sciex China

D. D. Dionysiou, J. Fang, V. K. Sharma, *Organizers*

D. A. Reckhow, T. Zhang, *Presiding*

1:30 Introductory Remarks.

1:35 ENVR **86.** Iron(III)-based metal organic frameworks as heterogeneous Fenton-like catalysts for organic pollutant degradation. C. Gao, **X. Quan**

2:00 ENVR **87.** Activation of manganese oxidants with bisulfite for enhanced oxidation of organic contaminants: The involvement of Mn(III). **X. Guan**

2:25 ENVR **88.** Role of dissolved Mn(III) in transformation of organic contaminants: Non-oxidative versus oxidative mechanisms. E. Hu, **F. He**

2:45 ENVR **89.** Cd(II) removal by manganese dioxide formed in situ from permanganate by thiosulfate: Influence of permanganate: Thiosulfate molar ratio. **P. Wang**, J. Jiang, J. Ma, H. Cheng, Z. Huang, B. Jia

3:05 Intermission.

3:20 ENVR **90.** Implementation of ferrate for drinking water treatment. **J.E. Tobiason**, D.A. Reckhow, J. Goodwill, Y. Jiang, J. Cunningham, X. Mai

3:45 ENVR **91.** Synergetic effect of the oxidation of fluoroquionolone antibiotics by a combined use of ferrate(VI) and peroxymonosulfate. M. Feng, Z. Wang, **V.K. Sharma**

4:10 ENVR **92.** Ferrate(VI) interactions with Natural Organic Matter (NOM) in drinking water treatment. **Y. Deng**, Y. Liang, C. Li, T. Waite

4:35 ENVR **93.** Withdrawn.

Section C

San Francisco Marriott Marquis

Salons 14/15

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Physical & Chemical Processes

Cosponsored by CHED

Financially supported by AEESP

M. J. McGuire, J. A. Pedersen, *Organizers*

F. L. Rosario, *Organizer, Presiding*

1:30 ENVR **94.** Granular activated carbon adsorption of specific organic compounds: A forty year retrospective of the 1979 National Academy of Science report. **R.S. Summers**

1:55 ENVR **95.** Fate of contaminants of emerging concern and geosmin in GAC biofilters: The roles of sorption and biodegradation. **R.M. Hozalski**, B. Ma, W. Arnold

2:20 ENVR **96.** Prediction of the adsorption capacities of organic pollutants on activated carbons in natural waters: Model development and validations. **T. Lin**, W. Bunmahotama, W. Hung

2:45 ENVR **97.** Predicting adsorption isotherms from adsorbent and adsorbate properties. **D. Knappe**, I. Mezzari, T. Speth

3:10 Intermission.

3:25 ENVR **98.** Can GAC be used to control priority unregulated DBPs in drinking water? **S.D. Richardson**, A.A. Cuthbertson, S.Y. Kimura, H.K. Liberatore, C. Joseph, D. Knappe, B.D. Stanford, R.S. Summers, E. Dickenson

3:50 ENVR **99.** Mn(II) oxidation in Fenton and Fenton-type systems: Identification of reaction efficiency and reaction products. **J. Pena**, C.M. Van Genuchten

4:15 ENVR **100.** Sequential manganese desorption–Adsorption in anthracite coal and silica sand filter media. **C.J. Gabelich**, F. Gerringer, C. Chou

4:40 ENVR **101.** Treating ion-exchange waste brines with a reduction-coagulation-filtration process using ferrous chloride. **N. Homan**, P.G. Green, **T.M. Young**

5:05 ENVR **102.** Ozone-derived NDMA in water reuse: Formation and mitigation. **E. Marti**, J.R. Batista, E. Dickenson

‡ *Cooperative Cosponsorship*

Section D

San Francisco Marriott Marquis
Golden Gate C1

Understanding Dissolved Organic Matter Reactivity: Honoring George Aiken, the DOM Whisperer

Y. Chin, D. M. McKnight, *Organizers*

K. Cawley, *Presiding*

1:30 ENVR **103.** X-ray Raman spectroscopy: An alternative approach for characterizing the carbon chemistry of organic matter. **E.J. O'Loughlin**, B. Mishra, W.T. Cooper, M. Tfaily, J. Jastrow, R.A. Gordon, M. Balasubramanian, K.M. Kemner

2:05 ENVR **104.** Forces holding organic matter molecules together: Involvement of exceptionally strong hydrogen bonds. **J.J. Pignatello**, J. Ni

2:30 ENVR **105.** Petroleum as a surrogate to unlock the compositional and structural continuum of dissolved organic matter. **D.C. Podgorski**, P. Zito, M.A. Tarr, R.G. Spencer

2:55 ENVR **106.** Electrochemical characterization of natural organic matter and its role as an electron transfer mediator in biogeochemical process. **P.G. Tratnyek**, A.S. Pavitt, J.T. Nurmi

3:20 Intermission.

3:30 ENVR **107.** Reactivity of natural organic matter determined by electrospray ionization coupled to Fourier transform ion cyclotron resonance mass spectrometry. **P.G. Hatcher**

4:05 ENVR **108.** Withdrawn.

4:30 ENVR **109.** PARAFAC analysis of irradiation- and oxidation-induced changes in fluorescent dissolved organic matter extracted from poultry litter. **K. Mangalgiri**, S. Timko, M. Gonsior, L.M. Blaney

4:55 ENVR **110.** Characterization of organic matter in wastewater from unconventional oil and gas production. **W.H. Orem**, M. Varonka, A. Bates, T. Schell, M. Engle

5:20 Concluding Remarks.

Section E

San Francisco Marriott Marquis
Sierra A

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

D. D. Dionysiou, G. Li Puma, D. Minakata, K. E. O'Shea, *Organizers*

X. He, X. Quan, *Organizers*, *Presiding*

1:30 ENVR **111.** Ozone regeneration of GAC for prolonged adsorption of brominated THMs. **X. He**, M. Elkouz, M. Inyang, E. Dickenson, E. Wert

2:05 ENVR **112.** Development of a computer-based prediction platform for transformation products during ozonation of micropollutants: Kinetics and mechanisms. **M. Lee**, L. Blum, E. Schmid, K. Fenner, U. von Gunten

2:30 ENVR **113.** Ozonation of substituted phenolic model compounds: Yields and toxicology of *p*-benzoquinones and polyphenols. **P.R. Tentscher**, B. Escher, N. Bramaz, K. Schirmer, M. Bourgin, U. von Gunten

2:55 ENVR **114.** Synergy during the oxidative degradation of organics using ozone combined a carbon nanotube electrochemical filter. **B.M. Chaves**, M.W. Dezotti, C.D. Vecitis

3:20 Intermission.

3:35 ENVR **115.** Mineralization as a mechanism for TOC removal: Study of ozone/ozone-peroxide oxidation using FT-IR. **S.A. Carr**

4:00 ENVR **116.** Comparison of the kinetics of the UV/chlorine and the UV/H_2O_2 processes in the degradation of PPCPs in simulated water and real water. **K. Guo**, Z. Wu, B. Yao, W. Song, C. Shang, J. Fang

4:25 ENVR **117.** Chloramine chemistry in AOP treated wastewaters. **L. Twight**, S.P. Mezyk, K.P. Ishida

4:50 ENVR **118.** Impact of the UV photolysis of monochloramine on 1,4-dioxane removal: New insights into potable water reuse. **S.D. Patton**, W. Li, K.D. Couch, S.P. Mezyk, H. Liu

Section F

San Francisco Marriott Marquis
Sierra B

Contaminants of Emerging Concern in Natural & Engineered Systems

Cosponsored by AGRO, ANYL and CEI

L. M. Blaney, A. J. Hernandez, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 ENVR **119.** Using fluorescent dissolved organic matter and contaminants of emerging concern to identify leaking wastewater collection systems. K. He, N. Rogers, **L.M. Blaney**

1:55 ENVR **120.** Transport and transformation of pharmaceuticals and other contaminants of emerging concern from wastewater discharge through surface water to drinking water intake and treatment. **E.T. Furlong**, S.T. Glassmeyer, D.W. Kolpin, M. Mills, M. Zimmerman, T. Jones-Lepp, M. Waldron

2:15 ENVR **121.** Contaminants of emerging concern in Portuguese rivers. **A.R. Ribeiro**, J. Sousa, M. Barbosa, M.R. Pereira, A.M. Silva

2:35 ENVR **122.** Estimating the Seattle, WA legal recreational cannabis market share using wastewater-based epidemiology. **D.A. Burgard**, J.R. Williams, C.J. Banta-Green

2:55 ENVR **123.** Use of chemical fate & transport research in environmental risk assessment. **E.M. Wong**, E.L. Libelo, M. Titcombe Lee

3:15 Intermission.

3:35 ENVR **124.** Bioaccumulation and estrogenicity of hormones and UV-filters in *Procambarus clarkii*. **K. He**, A. Timm, L.M. Blaney

3:55 ENVR **125.** Mixtures of contaminants of emerging concern commonly detected in Great Lakes tributaries reduce reproductive potential in wild and laboratory exposed fishes. **H.L. Schoenfuss**, L.C. Wang, Z.G. Jorgenson, S.J. Choy, J. Banda, D.J. Gefell, M. Annis, W. Tucker, S.M. Elliott, M.E. Brigham

4:15 ENVR **126.** Spatio-temporal occurrence, bioaccumulation, and trophic transfer of select contaminants of emerging concern in a semi-arid river influenced by snowmelt. **S. Haddad**, C. Scott, B. Burket, S. James, G. Saari, L. Kristofco, K. Chambliss, M. Luers, C. Rogers, B.W. Brooks

4:35 ENVR **127.** Evaluating the impacts of metformin and mixtures of other dominant contaminants of emerging concern in Milwaukee Estuary and Lake Michigan. **R. Klaper**, J. Crago, N. Niemuth

4:55 ENVR **128.** Application of water cooling towers for monitoring environmental releases of tritium. **R. Brigmon**, D. Kaplan, C. Milliken, T. Jannik, H.A. Brant, B. Viner

5:15 Concluding Remarks.

Section G

San Francisco Marriott Marquis
Sierra C

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Cosponsored by ANYL

T. Anumol, R. Marfil-Vega, T. M. Young, *Organizers*, *Presiding*

1:30 ENVR **129.** Unknown microcystin screening using LC-MS/MS, triggered information dependent acquisition, and confirmation by Q-TOF analysis with Personal Compound Database and Library. **R.A. Trenholm**, B. Vanderford

1:55 ENVR **130.** Expanding targets of UPLC-ToF-MS metabolomics and ^{15}N labeling in Cyanobacterial Harmful Algal Bloom (CHAB) research: Microcystins and beyond. **W.K. Strangman**, A. Stewart, J.L. Wright

2:45 ENVR **131.** Method development of a 2D LC HRMS extraction and detection method for organophosphors flame retardants in environmental water samples. **L. Mullin**, M. Mella, C. Mallet, D. Stevens, I. Ericston Jogsten, G. Cleland

3:10 ENVR **132.** Identification of emerging contaminants from the waste water influenced Tioga River using high resolution accurate mass LC/MS and statistical analysis. **J. Zweigenbaum**, T. Anumol, L. Kennedy

3:35 Intermission.

3:50 ENVR **133.** Comprehensive workflow for micropollutant identification and prioritization using HR/AM tandem mass spectrometry and cheminformatics. **L. Ferguson**, G.J. Getzinger

4:15 ENVR **134.** Smart target method development for detection of antiviral compounds in aqueous environmental samples based on suspect screening and HRMS. **D. Barcelo**, B. Zonja, J. Guillen, M. Lopez de Alda

4:40 ENVR **135.** LC-HRMS data combined with cluster analysis to compare wastewater treatment efficiency. **J.E. Schollée**, M. Bourgin, C.S. McArdell, J. Hollender

5:05 ENVR **136.** Using the US EPA's CompTox Dashboard to support identification and screening of emerging organic contaminants in the environment. **A. McEachran**, J. Sobus, S. Newton, M. Strynar, A.J. Williams

Section H

San Francisco Marriott Marquis
Sierra J

Green Chemistry & the Environment

Cosponsored by CEI

Financially supported by AEESP

A. M. Balu, R. Luque, *Organizers*

S. O. Obare, *Organizer, Presiding*

T. Dittrich, D. Vardon, *Presiding*

1:30 ENVR **137.** Withdrawn.

1:50 ENVR **138.** Aluminum-cycle ion exchange process for hardness removal: A new approach for sustainable softening. **M. German**, J. Li, A.K. Sengupta

2:10 ENVR **139.** Chlorate formation in on-site hypochlorite generators: Dependence on pH-level, temperature and storage time. **L. Kriem**, R.N. Biagioni

2:30 ENVR **140.** Alpha-pinene isomerization over silica supported heteropolyacids. **L. Frattini**, M. Isaacs, C.M. Parlett, K. Wilson, G. Kyriakou, A.F. Lee

2:50 ENVR **141.** Bandgap engineering of $Bi_2Ti_2O_7$ through foreign ion incorporation via solution combustion synthesis. **G.F. Samu**, K. Rajeshwar, C. Janaky

3:10 Intermission.

3:25 ENVR **142.** Mesoporous manganese oxide catalyzed aerobic oxidative coupling of anilines to aromatic azo compounds. **B. Dutta**, S.L. Suib

3:45 ENVR **143.** Effect of elevated atmospheric CO_2 on arsenic uptake in different ecotypes of *Arabidopsis thaliana*: Implications for phytoremediation efficacy. **V. Fernandez-Alos**, J. Barnaby, M. Tomecek, E. Codling, L. Ziska

4:05 ENVR **144.** Electrochemical generation of H_2O_2: Development of a reactor with carbon catalysts for portable low-cost water purification. **Z. Chen**, S. Chen, S. Siahrostami, P. Chakthranont, C. Hahn, D. Nordlund, D. Sokaras, J.K. Norskov, Z. Bao, T.F. Jaramillo

4:25 ENVR **145.** Biopolymers as treatment agents for crude oil-contaminated seawater. **T. Ameh**, R. Srinivasan, C. Thompson, B. Bellows, M. Murphy

4:45 ENVR **146.** Bio-inspired doped calcium carbonate particles for effluent removal from waste water. **H. Ramesh**, K. Radhakrishnan, S. Kumar Nadar, A. Raichur

5:05 ENVR **147.** Waste shell biorefinery: Dream or reality? **N. Yan**

Section I

San Francisco Marriott Marquis
Sierra K

Integrated & Sustainable Environmental Remediation

Cosponsored by CEI

S. K. Brar, R. Galvez, *Organizers*

M. Cledon, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **148.** Effect of synergistic interaction between Ce and Mn on the CO_2 capture of calcium-based sorbent: Textural properties, ability of donating electrons, and generation of oxygen vacancy. **H. Guo**, J. Feng, Y. Zhao, X. Ma, **S. Wang**

1:55 ENVR **149.** Chemical and adsorptive characterization of solids to capture greenhouse gases under standard conditions of temperature and pressure. **B. Delgado**, A. Avalos Ramirez, R. Lagacé, A. Giroir-Fendler, S. Godbout

2:15 ENVR **150.** Biodegradation of hexabromocyclododecane by *Rhodopseudomonas palustris* sp. **R. Wang**, T. Chang, Y. Peng, Y. Shih

2:35 ENVR **151.** Withdrawn.

2:55 ENVR **152.** Assessment of changes in ecotoxicity of dredged marine sediment by sediment treatments for TPH removal. **K. Kim**, G. Joo, B. Jeong, K. Nam, Y. Choi

3:15 Intermission.

3:30 ENVR **153.** Sediment contaminant accumulation in stormwater catchment basins: New implications for management guidelines. **V. Craver**, L. Schifman, V. Kasaraneni, T. Boving

3:50 ENVR **154.** Advanced study of unconventional oil behaviour in regard to surface water oil spills. **R. Galvez**

4:10 ENVR **155.** Integrated municipal solid waste management: Renewable energy and activated carbons for leachate treatment. **J.L. Goldfarb**, **C. Gopu**

4:30 ENVR **156.** Removal of chlortetracycline from water using immobilized laccase onto adsorptive membrane. **M. Taheran**, M. Naghdi, S.K. Brar, E.J. Knystautas, M. Verma, R.Y. Surampalli, J.R. Valero

4:50 ENVR **157.** Electrochemical deposition for the recovery and separation of metals: A novel approach for reclaiming rare earth and specialty elements from industrial waste and processing streams. M. O'Connor, R. Coulthard, **D. Plata**

5:10 ENVR **158.** Withdrawn.

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

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Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Sponsored by GEOC, Cosponsored by COLL and ENVR

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Sponsored by CATL, Cosponsored by COLL and ENVR

MONDAY MORNING

Section A

San Francisco Marriott Marquis
Salons 10/11

Tribute to Jerry Schnoor

J. G. Burken, D. M. Cwiertny, C. L. Just, *Organizers*, *Presiding*

8:00 ENVR **159.** Nanoparticle surface affinity as a predictor of nanoparticle fate, biouptake and trophic transfer. **M. Wiesner**, N. Geitner, A. Turner, N. O'Brian

8:30 ENVR **160.** Analytical and toxicological studies of emerging water disinfection byproducts halobenzoquinones. **X. Li**, W. Wang, J. Li, G. Huang, L. Blackstock-Jmaiff, I. Vander Meulen, J. Zhang

8:50 ENVR **161.** DLVO energy of interaction of macromolecule-coated silver nanoparticles. **T. Zhu**, D. Lawler

9:10 ENVR **162.** Waste acid as the energy source for desalination, softening and mechanical work. **A.K. Sengupta**, M. German

9:30 Intermission.

9:45 ENVR **163.** Phytoforensic methods from the air: Hyperspectral Image (HSI) comparison of plant responses to energetics exposure and drought stress. P. Manley, A. Ghulam, Z. Yin, M.Y. Berezin, C.E. Johnson, **J.G. Burken**

10:15 ENVR **164.** Differential response of *Arabidopsis thaliana* to Polychlorinated Biphenyls (PCBs) and their hydroxylated metabolites (OH-PCBs). **B. VanAken**, S. Subramanian, J.L. Schnoor

10:35 ENVR **165.** Photolysis of 2,4-dinitroanisole and its metabolites in *Arabidopsis* leaves. **H. Schroer**, C.L. Just

10:55 ENVR **166.** Innovations in passive sampling for bioavailable contaminants in sediments. **D.D. Reible**, X. Shen, M. Rakowska, S. Yan

Section B

San Francisco Marriott Marquis
Salons 12/13

Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in honor of Prof. Jun Ma

Advanced Oxidation Processes

Financially supported by Sciex China

D. D. Dionysiou, J. Fang, V. K. Sharma, *Organizers*

Y. Lee, W. Mitch, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **167.** Understanding chloramine-driven photochemistry for water reuse applications. **H. Liu**

8:30 ENVR **168.** Transformation of benzophenone-4 by chlorine, chloramine, and UV/chlorine. **J. Lu**, Y. Ji

8:50 ENVR **169.** Comparison of UV/free chlorine, UV/monochloramine, and UV/hydrogen peroxide advanced oxidation processes for contaminant degradation under scenarios relevant to potable reuse. **Y. Chuang**, W. Mitch

9:10 ENVR **170.** Investigation of the iopamidol degradation by UV/chlorine. **X. Kong**, J. Jiang, J. Ma, J. Fang

9:30 ENVR **171.** Reactive chlorine species significantly contributes to the degradation of trimethoprim in the UV/chlorine process. **Z. Wu**, K. Guo, C. Shang, J. Fang

9:50 Intermission.

10:05 ENVR **172.** Radical chemistry of the UV/chlorine process on the degradation of micropollutants in water treatment. **J. Fang**, K. Guo, Z. Wu, M. Pan, Z. Ren, C. Shang

10:30 ENVR **173.** Formation and conversion of sulfate radical and hydroxyl radical in UV/peroxymonosulfate system. **Y. Guan**, J. Ma

10:55 ENVR **174.** Degradation of chlorophenol by hydroxylamine and peroxymonosulfate. **L. Chen**, J. Zhang, P. Wang, Y. Huang, B. Wu

11:15 ENVR **175.** Kinetic study of hydroxyl and sulfate radical-mediated oxidation of pharmaceuticals in wastewater effluents. **L. Lushi**, B. Yao, S. Hou, J. Fang, S. Yan, W. Song

11:35 ENVR **176.** Denitration and renitration processes in sulfate radical-based oxidation of nitroaromatic compounds. **Y. Ji**

Section C

San Francisco Marriott Marquis
Salons 14/15

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Physical & Chemical Processes

Cosponsored by CHED

Financially supported by AEESP

J. A. Pedersen, F. L. Rosario, *Organizers*

M. J. McGuire, *Organizer, Presiding*

8:00 ENVR **177.** Efficient anaerobic membrane bioreactor treatment of municipal wastewater for energy and biosolids reduction. **P. McCarty**, J. Kim, C. Shin, J. Bae

8:25 ENVR **178.** Optimization of urban groundwater recharge systems that infiltrate combined stormwater and recycled water through surface spreading basins. J.L. Bradshaw, **R.G. Luthy**

8:50 ENVR **179.** Thermal air oxidation during biomass char formation and its effects on adsorption of organic compounds. **J.J. Pignatello**

9:15 ENVR **180.** Modeling organic contaminant sorption by biochar and activated carbon: Insights into concentration independent removal and isotherm curvature. **K. Shimabuku**, J. Paige, M. Luna Aguero, R.S. Summers

9:40 ENVR **181.** Advanced oxidation-driven transformation of Contaminant Candidate List (CCL_3) compounds in drinking water. **K. Linden**, U. von Gunten, H. Mestankova, A.M. Parker, S. Canonica, K. Schirmer

10:05 Intermission.

10:20 ENVR **182.** Toxicity profiles and metastable disinfection byproducts. **D.A. Reckhow**, Y. Yu

10:45 ENVR **183.** Regeneration of strong base ion exchange resin for hexavalent chromium removal. **J.A. Korak**, M. Arias-Paic

11:10 ENVR **184.** Options for hydrogen sulfide remediation in complex water matrices. **L.E. Schweitzer**

11:35 ENVR **185.** Water disinfection: From laboratory bench to full scale. Where we are and where we need to go. **C.N. Haas**, B. Farouk, W. Wei

Section D

San Francisco Marriott Marquis
Golden Gate C1

Understanding Dissolved Organic Matter Reactivity: Honoring George Aiken, the DOM Whisperer

Y. Chin, D. M. McKnight, *Organizers*

R. M. Cory, *Presiding*

8:00 Introductory Remarks.

8:10 ENVR **186.** What can simple measurements of DOM tell us when made in new ways? **B. Bergamaschi**

8:45 ENVR **187.** Characterization of dissolved organic matter during municipal wastewater treatment. **C.K. Remucal**, A. Maizel, S. Berg

9:10 ENVR **188.** Characterization of fluorescent DOM in textile dyeing wastewater. **C. Cheng**, J. Wu, B. Liu, J. Tang, K.M. Saleem

9:35 ENVR **189.** Reactivity towards N-Nitrosamines of bulk and trace organics of wastewater origin. **P.K. Westerhoff**, J. Rice, D. Hanigan, A. Dotson

10:00 Intermission.

10:10 ENVR **190.** National Ecological Observatory Network (NEON): Dissolved organic matter quantity and quality. **K. Cawley**

10:45 ENVR **191.** Relationships between microbial activity, nutrients, and organic matter chemistry in urban-impacted rivers. **R.S. Gabor**, R. Smith, J.F. Shah, P.D. Brooks

11:10 ENVR **192.** Concentration-discharge relationships during the recession of an extreme flood in the Boulder Creek Watershed: Patterns of lithologic solute concentrations contrast with decreases in concentration and changes in chemical quality of dissolved organic material. **G. Rue**, D.M. McKnight, N. Rock, R.S. Gabor, M. Tfaily

11:35 ENVR **193.** Pb and Hg mobilization by dissolved organic matter in an ombrotrophic peatland. **J. Jeremiason**, S.D. Sebestyen, E. Baumann, E. Seelen, A. Agather

‡ *Cooperative Cosponsorship*

Section E

San Francisco Marriott Marquis
Sierra E

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

D. D. Dionysiou, X. He, G. Li Puma, D. Minakata, X. Quan, *Organizers*

K. E. O'Shea, *Organizer, Presiding*

A. Pintar, *Presiding*

8:00 ENVR **194.** Improved electron-hole separation/migration in anatase TiO_2 nanotube/reduced graphene oxide composites for efficient photocatalytic degradation of bisphenol A. G. Zerjav, S. Arshad, P. Djinovic, I. Junkar, J. Kovac, J. Zavasnik, **A. Pintar**

8:35 ENVR **195.** Nitrogen doped porous carbon with peroxymonosulfate activation capability for effective water treatment. **G. Wang**, X. Quan, S. Chen, H. Yu

9:00 ENVR **196.** Post-illumination activity of SnO_2 nanoparticle-decorated Cu_2O nanocubes by H_2O_2 production in dark from photocatalytic memory. L. Liu, W. Sun, W. Yang, **Q. Li**, J. Shang

9:25 ENVR **197.** Photocatalytic removal of triclosan and triclocarban by zinc oxide and nitrogen-doped reduced graphene oxide. **M. Hwangbo**, T. Alivio, Y. Shi, S. Banerjee, K. Chu

9:50 Intermission.

10:05 ENVR **198.** Efficient contaminant degradation by hydrogen peroxide activated graphite-supported Fe-TAML catalyst. **Y. Chang**, C. Miller, D. Waite

10:30 ENVR **199.** Evaluations of biotrickling filters for the removal of mixtures of trihalomethanes under two environmental conditions. **B. Mezgebe**, G. Sorial, E. Sahle-Demessie

10:55 ENVR **200.** Reactivity of trichloramine (NCl_3) with amino acids prior to advanced oxidation process treatment. **L. Watts**, J. Gleason, S.P. Mezyk, K.P. Ishida

11:20 ENVR **201.** Photocatalytic activity enhancement of ZnO thin films under visible light using Bi_2O_3 dots. **J.C. Medina**, N.S. Portillo-Veléz, M. Bizarro, A. Hernández-Gordillo, S.E. Rodil

Section F

San Francisco Marriott Marquis
Sierra B

Contaminants of Emerging Concern in Natural & Engineered Systems

Cosponsored by AGRO, ANYL and CEI

L. M. Blaney, A. J. Hernandez, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ENVR **202.** Role of Mn-oxide controlling the pathways of glyphosate degradation. **H. Li**, D. Jaisi

8:55 ENVR **203.** Kinetic study of thermal monochloramine reactions with nitrogenous compounds. **J. Gleason**, S.P. Mezyk, K.P. Ishida

9:15 ENVR **204.** Impact of sulfate ions on electrochemical oxidation of recalcitrant organic compounds using boron-doped diamond anodes. **A. Farhat**

9:35 ENVR **205.** Effect of chlorination and chloramination on the removal of micropollutants in wastewater treatment plants. N. Bilgin Saritas, E. Aydin, **E. Pehlivanoglu Mantas**

9:55 Intermission.

10:15 ENVR **206.** Investigation of radical chlorine species reactions in advanced oxidation processes. S.P. Mezyk, **J. Castillo**, J. Gleason, K.P. Ishida

10:35 ENVR **207.** Coupled titanium dioxide photocatalysis and filtration to mitigate organic matter and estrogens. C. Johnson, P.J. McNamara, **B. Mayer**

10:55 ENVR **208.** Kinetic study of organophosphate flame retardant reactions with hydroxyl radicals. **S.P. Mezyk**

11:15 ENVR **209.** Regulated and unregulated halogenated disinfection byproduct formation from chlorination of high salinity groundwaters. **A. Szczuka**, W. Mitch

11:35 Concluding Remarks.

Section G

San Francisco Marriott Marquis
Sierra C

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Cosponsored by ANYL

T. Anumol, R. Marfil-Vega, T. M. Young, *Organizers*, *Presiding*

8:00 ENVR **210.** Characterization of nitro-substituted polycyclic aromatic hydrocarbons from standard diesel particulate matter using liquid chromatography orbitrap mass spectrometry. **M.S. Bataineh**

8:25 ENVR **211.** Identifying trace environmental contaminants in CO_2 capture solvents from coal-fired power plants using high resolution Time-of-Flight Mass Spectrometry (TOF-MS). **J.G. Thompson**, S. Bhatnagar, K. Liu

8:50 ENVR **212.** Utilization of soft and hard ionization techniques with 2-dimensional gas chromatography and high-resolution mass spectrometry for unknown identification in hydraulic fracturing fluid, flowback and produced water samples. **J. Rosenblum**, K. Linden, A.J. Dane, E. Thurman, I. Ferrer

9:15 ENVR **213.** Nontarget analysis of hydraulic fracturing flowback waters throughout the fracturing process using LC-QToF-MS. **K. Oetjen**, P.C. Winkler, T.Y. Cath, J. Blotevogel, T. Borch, R. Young, C.P. Higgins

9:40 ENVR **214.** Identifying endocrine disrupting compounds in treated sewage sludge using non-targeted LC/MS/MS and CALUX cell-based bioassays. **G. Pecora**, T.M. Young, T. Anumol

10:05 Intermission.

10:20 ENVR **215.** Exploring the great unknown: Role of NTA in ensuring water safety. **S.A. Snyder**

10:45 ENVR **216.** Resolving masses and bottlenecks for long-term LC-MS monitoring with the enviMass workflow version 3.2. **M.J. Loos**, S. Ruppe, J. Mazacek, H. Singer

11:10 ENVR **217.** Suspect and non-target screening of organic contaminants In stormwater runoff and exposed fish. **E.P. Kolodziej**, B. Du, J. Lofton, J. McIntyre, N. Scholz, J. Davis, J.E. Baker

11:35 Discussion.

11:55 Concluding Remarks.

Section H

San Francisco Marriott Marquis
Sierra J

Sulfidation of Metal-Based Engineered & Natural Nanomaterials: Implications for Their Fate & Effects in the Environment

Y. Bi, P. K. Westerhoff, *Organizers*

D. Fan, P. G. Tratnyek, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **218.** Rates, mechanisms, and impacts of sulfidation of metal and metal oxide nanoparticles on their fate and effects in wastewater treatment plants and freshwater wetland mesocosms. **G. Lowry**, J.P. Stegemeier

8:35 ENVR **219.** Formation and oxidative stability of metal sulfide nanoparticles and 2D nanosheets. Z. Wang, Y. Zhang, E. Gray, A. Peterson, **R. Hurt**

9:05 ENVR **220.** Dissolution behavior of silver nanoparticles and formation of secondary sulfidated silver nanoparticles in municipal wastewater by single particle ICP-MS. **S. Ghoshal**, M.M. Azodi

9:25 ENVR **221.** Silver nanoparticles fate at the solution/biofilm/mineral interface. **M. Desmau**, G. Alexandre, C. Levard, G. Ona-Nguema, V. Vidal, M. Auffan, P.J. Eng, M.F. Benedetti

9:45 ENVR **222.** Electroanalytical methods in characterization of metal sulphide nanoparticles in water environment. M. Marguš, I. Coha, M. Lovrić, **I. Ciglenecki**

10:05 Intermission.

10:20 ENVR **223.** Spectroscopic investigation of the mechanism and kinetics of the sulfidation of Fe^{III}-(oxyhydr)oxide nanoparticles. **N. Kumar**, V. Noël, J. Pacheco, K. Maher, G.E. Brown

10:50 ENVR **224.** Oxidation of synthetic iron(II) monosulfide at circumneutral pH when exposed to aerobic conditions: Fe-mineral transformations and oxidizing capacity of the system. **C. Miller**, R. Collins, D. Waite

11:10 ENVR **225.** Reductive immobilization of hexavalent chromium by polysulfide-reduced iron (hydro) oxides. **M. Shi**, J. Li, J.S. Zheng

11:30 ENVR **226.** Trichloroethene dechlorination by mechanochemically sulfidated zero valent iron: Reaction pathway, kinetics and electron efficiency. Y. Gu, **F. He**

Section I

San Francisco Marriott Marquis
Sierra K

Advances & Applications in Water Sensing Technologies for Drinking Water, Re-Use, Agri-Tech & Research

C. Moldaenke, W. Zhang, *Organizers*

M. E. Romero-Gonzalez, P. L. Schorr, *Organizers*, *Presiding*

8:00 ENVR **227.** Advances in sensing technologies for water monitoring. **M.E. Romero-Gonzalez**

8:20 ENVR **228.** Fluorescence spectroscopy: A tool to monitor presence of contaminants in water reuse systems. **J. Wasswa**, N. Mladenov

8:40 ENVR **229.** Highly stable SERS nanoprobes for pH detection in confined water environment. **H. Wei**, M. Willner, L.C. Marr, P.J. Vikesland

9:00 ENVR **230.** Ultra-trace electrochemical sensing of heavy metals using nanostructured bismuth doped carbon complex: Real time on site environmental application. **K.M. Zeinu**

9:20 ENVR **231.** Optimization of coagulation process for the removal of Natural Organic Matter (NOM) characterized by Excitation-Emission Fluorescence Matrix (EEM) via 2-level Full Factorial Design (FFD) methodology. **R.C. Go**, C. Kan, M.G. de Luna

9:40 ENVR **232.** Validation and optimization of an alternative method for NDMA analysis requiring less time, cost, and sample volume. **S. Roback**, M.H. Plumlee, H. Kodamatani, T. Fujioka

10:00 Intermission.

10:15 ENVR **233.** Development of NanoAptamer assay and portable analyzer for the detection of bisphenol A. **H. Lim**, E. Lee, S. Lee, B. Chua, A. Son

10:35 ENVR **234.** Conjugated molecule based resistive sensor for microbial detection in water with *E. coli* as a case study. **A.N. Mallya**, D.C. Ramamurthy

10:55 ENVR **235.** Molecular imprinted composite sol-gel layers for conductometric sensing of environmental toxins. **A. Mujahid**, **T. Hussain**, H. Munir

11:15 ENVR **236.** Fluorometer using the pigment phycocyanin as an early warning system for the appearance of difficult to treat cyanobacterial T&O compounds and cyanotoxins in comparison to UV-EEM online parameters as amino acids. **C. Moldaenke**, H. Dahlhaus, W. Schmidt, M. Wagner, S. Kueppers, **P.L. Schorr**

11:35 ENVR **237.** Withdrawn.

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Sponsored by GEOC, Cosponsored by COLL and ENVR

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

Advances in Treatment Processes for Metals & Metalloids

Sponsored by GEOC, Cosponsored by ENVR

TECHNICAL PROGRAM

Chemistry & Physical Chemistry of Thermal Processes for the Circular Carbon Economy

Sponsored by CELL, Cosponsored by ENFL and ENVR

Elucidation of Mechanisms & Kinetics on Surfaces

Surface Science

Sponsored by CATL, Cosponsored by COLL and ENVR

MONDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Salons 10/11

Tribute to Jerry Schnoor

J. G. Burken, D. M. Cwiertny, C. L. Just, *Organizers*, *Presiding*

1:00 ENVR **238.** Withdrawn

1:30 ENVR **239.** Phytoforensic methods to affirm impacts of endophytoc degradation in field phytoremediation process. S.L. Doty, M.J. Blaylock, J. Freeman, C. Cohu, **J.G. Burken**, A. Simon, J. Isebrands

1:55 ENVR **240.** Health risk for residents via inhalation exposure to particle-bound hydrophobic organic compounds and heavy metals in a typical e-waste recycling zone. P. Luo, C. Huang, L. Bao, S. Li, **E. Zeng**

2:20 ENVR **241.** Withdrawn.

2:45 Intermission.

3:00 ENVR **242.** Trees as indicators of vapor intrusion risk. **J.L. Wilson**, M. Limmer, V. Samaranayake, J. Schumacher, J.G. Burken

3:25 ENVR **243.** Use of environmental fate models in U.S. EPA TSCA new chemicals assessments. **M. Card**, E.L. Libelo, K. Mayo-Bean, D. Lynch

3:50 ENVR **244.** Arsenic in geogenic soil from Hong Kong: Speciation, mobilization, and bioaccessibility. J. Cui, Y. Zhao, J. Li, D. Tsang, C. Poon, T. Chan, W. Wang, **X. Li**

4:15 ENVR **245.** Modeling ion exchange equilibria in cross-linked cationic surfactant nanoparticle solutions. **M. Chen**, C.T. Jafvert

4:40 Panel Discussion.

Section B

San Francisco Marriott Marquis

Salons 12/13

Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in honor of Prof. Jun Ma

Heterogeneous Catalytic Oxidation Processes in Water & Wastewater Treatment

Financially supported by Sciex China

J. Fang, V. K. Sharma, *Organizers*

D. D. Dionysiou, *Organizer, Presiding*

T. An, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR **246.** Three-dimensional MnO_2 porous hollow microspheres for enhanced activity as ozonation catalysts in water treatment. **C. He**, Y. Huang, W. Xu, X. Tan

1:30 ENVR **247.** Enhanced degradation of organic micropollutants via heterogeneous photo-Fenton reactions on α-FeOOH. **W. Zhang**, G. Zhang, P. Wang

1:55 ENVR **248.** Comparison of catalytic ozonation by $LaFeO_3$ and $LaCoO_3$: Benzotriazole degradation, elimination of bromate andreaction mechanism. **Y. Zhang**, Y. Xia, Q. Li, B. Xu, F. Qi

2:15 ENVR **249.** Visible light activated nanosized bismuth titanates for photocatalytic degradation of bisphenol A. **M.K. Patil**, B. Ren, M. Nadagouda, D.D. Dionysiou

2:35 Intermission.

2:50 ENVR **250.** Enhanced visible-light-responsive photocatalytic degradation of emerging pollutants by $ZnFe_2O_4$/TiO_2 heterostructures. **R. Doong**

3:15 ENVR **251.** $LaFeO_3$ perovskite as a nanocatalyst for diclofenac degradation by heterogeneous activation of oxone process: Efficiency and mechanism. **Y. Rao**

3:40 ENVR **252.** Efficient degradation of carbamazepine in aqueous solution by bismuth oxybromide-activated peroxide oxidation. X. Liu, **J. Li**, T. Zhang

4:00 ENVR **253.** BiOI microspheres for pre-treatment of winery wastewater. **A. Mera**

4:20 ENVR **254.** Degradation of dimethyl phthalate by peroxomonosulfate activated with Zn-NiOx. **G. Zhang**, J. Zhang, **P. Zhou**, Y. Zhang

Section C

San Francisco Marriott Marquis

Salons 14/15

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Characterization of Natural Organic Matter

Cosponsored by CHED

Financially supported by AEESP

M. J. McGuire, F. L. Rosario, *Organizers*

J. A. Pedersen, *Organizer, Presiding*

1:00 ENVR **255.** Abbreviated review of photochemistry of natural organic matter then (1989) and now (2017). **W.J. Cooper**, B.A. Cottrell

1:25 ENVR **256.** Environmental photochemistry of organic matter. **F.L. Rosario**

1:50 ENVR **257.** Assessing dissolved organic matter photo-reactivity in a subtropical wetland ecosystem: Correlations between optical properties, antioxidant capacity, and the photochemical formation of reactive intermediates. **G. McKay**, W. Huang, C. Romera-Castillo, F.L. Rosario, R. Jaffe

2:15 ENVR **258.** Post treatment challenges at advanced potable reuse plants: Corrosion, metals mobilization and the reappearance of disinfection byproducts. **S. Roback**, K.P. Ishida, M.H. Plumlee, J. Dadakis, W. Mitch, S.E. Fendorf, D. Hokanson

2:40 Intermission.

2:55 ENVR **259.** Isolation and characterization of natural organic matter from Pony Lake, Antarctica. **E.M. Perdue**, S. Driver

3:20 ENVR **260.** NOM: From unfiltered supplies to water boil orders. **W.C. Becker**

3:45 ENVR **261.** Impact of pre-oxidation on the removal of regulated and emerging disinfection byproducts by activated carbon. **E.M. Verdugo**, M. Gifford, S.D. Richardson, R.S. Summers, B.D. Stanford, E. Dickenson

4:10 ENVR **262.** Characterization and monitoring of dissolved organic matter at drinking water treatment plants: Methods and application. **M. Philibert**, C. Cazin, F. Zraick

Section D

San Francisco Marriott Marquis

Golden Gate C1

Understanding Dissolved Organic Matter Reactivity: Honoring George Aiken, the DOM Whisperer

D. M. McKnight, *Organizer*

Y. Chin, *Organizer, Presiding*

1:00 ENVR **263.** Watershed tea in arctic lakes: Comparing carbon chemistry and cycling in red zinger vs. chamomile waters. **R.M. Cory**, C.P. Ward, J. Bowen, A. Trusiak, L. Treibergs

1:35 ENVR **264.** Permafrost dissolved organic matter leachability and reactivity in the presence of various solutions from an Alaskan Sub-Arctic watershed. **K.R. Gagne**, J.J. Guerard

2:00 ENVR **265.** Relating the reactivity of triplet excited states of dissolved natural organic matter to organic matter quality and land cover in mixed-use watersheds. A.J. McCabe, **W. Arnold**

2:25 ENVR **266.** Cross-scale advances in CDOM biogeochemistry: From molecular to ecoregional perspectives. **P.L. Brezonik**, C.G. Griffin, J.C. Finlay, L.G. Olmanson, R.M. Hozalski, B.J. Allen, W. Arnold, M.E. Bauer

2:50 Intermission.

3:00 ENVR **267.** From the Antarctic to the Arctic: An expeditionary approach to the environmental chemistry and reactivity of dissolved organic matter. **D.M. McKnight**

3:35 ENVR **268.** Location matters: Groundwater flow direction (recharge vs. discharge) controls DOM and DIN gradients and cycling in the bed sediments of a groundwater flow-through lake. **R.L. Smith**, D.B. Kent, D.R. LeBlanc, J. Bohlke, D.A. Repert, D. Stoliker, R. Hull, T.D. McCobb, J. Underwood, C. Conaway, A.P. Reed

4:00 ENVR **269.** Evidence for conservative transport of dissolved organic carbon in major river basins in Maine. **T. Huntington**, C. Roesler, G. Aiken

4:25 ENVR **270.** Is disturbance mobilizing or creating the aged carbon exported in streams? **R.T. Barnes**, D. Butman, P. Raymond, H. Wilson

4:50 Concluding Remarks.

Section E

San Francisco Marriott Marquis

Sierra A

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

D. D. Dionysiou, G. Li Puma, D. Minakata, K. E. O'Shea, X. Quan, *Organizers*

X. He, *Organizer, Presiding*

T. An, R. Pupo Nogueira, *Presiding*

1:00 ENVR **271.** Application of photo-fenton process for the degradation of antibiotics and disinfection of anaerobic pre-treatmed hospital effluent. J.A. Perini, A.L. Tonetti, **R. Pupo Nogueira**

1:35 ENVR **272.** Analogies and differences between bacterial and viral inactivation during photo-Fenton treatment of wastewater. **S. Giannakis**, C. Pulgarin

2:00 ENVR **273.** Effect of porous structure on the heterogeneous Fenton oxidation regeneration of magnetic carbon. **Y. Xiao**, J.M. Hill

2:25 ENVR **274.** Coupling photocatalysts and ferrate oxidation: Towards an innovative solution for wastewater treatment. **T. Pigot**

2:50 Intermission.

3:05 ENVR **275.** Photochemical and photocatalytic transformation mechanism and risk assessment of typical synthetic musks in water: Theoretical study. G. Yanpeng, G. Li, **T. An**

3:40 ENVR **276.** Theoretical study of the reaction of OH radicals with benzoic acid in the gas and aqueous phase. **C. Wu**, A. De Visscher, I. Gates

4:05 ENVR **277.** Activation of Fe-tpena by hydrogen peroxide to form an unselective strong oxidant at circumneutral pH. **C. Miller**, Y. Chang, D.P. de Sousa, C.J. McKenzie, D. Waite

4:30 ENVR **278.** Degradation mechanisms of algal odorants of β-cyclocitral and β-ionone during UV photolysis and UV/chlorination reactions. T. Kim, T. Kim, M. Kim, **K. Zoh**

Section F

San Francisco Marriott Marquis

Sierra B

Contaminants of Emerging Concern in Natural & Engineered Systems

Cosponsored by AGRO, ANYL and CEI

L. M. Blaney, A. J. Hernandez, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR **279.** Novel method for the quantification of the total *N-nitrosamines* concentration (TONO) in water. **F. Breider**, U. von Gunten

1:25 ENVR **280.** Formation of vegetable-derived disinfection byproducts. **Y. Komaki**, J. Choe, W. Mitch

1:45 ENVR **281.** NDMA precursor transformation and identification during reverse osmosis and UV/peroxide water treatment for indirect potable reuse. **D. Hanigan**, I. Ferrer, E. Thurman, S. Roback, K.P. Ishida, M.H. Plumlee, P.K. Westerhoff

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

2:05 ENVR **282.** Study of N-Nitrosodimethhyleamine (NDMA) formation in the untreated surface water using preformed chloramines. **S. Prabakar**, F. Samadi, A. Kruzic

2:25 Intermission.

2:45 ENVR **283.** Fate of micropollutants in high-capacity wastewater treatment plants in Istanbul metropolitan area. S.C. Tuzun, **E. Aydin**, E. Pehlivanoglu Mantas

3:05 ENVR **284.** Biotransformation of trace oganic compounds in aerobic, anaerobic and anoxic conditions. **N. Lm**, B. Vanderford, E. Dickenson, D. McAvoy

3:25 ENVR **285.** Prevalence and elimination of extracellular antibiotic resistance genes in five full-scale membrane reactors. **S. Zhou**, Y. Wang

3:45 ENVR **286.** Roles played by ammonia oxidizers of a nitrifying activated sludge community in micropollutant biotransformation. **Y. Men**, P. Han, S. Archermann, Y. Yu, D.E. Helbling, D.R. Johnson, M. Wagner, K. Fenner

4:05 ENVR **287.** Inhibition of the cometabolic transformation of 1,4-dioxane by *Rhodococcus rhodochrous* 21198 grown on isobutane. **M.F. Azizian**

4:25 Concluding Remarks.

Section G

San Francisco Marriott Marquis

Sierra C

Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences

Cosponsored by ANYL and CHED

Financially supported by AEESP

M. A. Benvenuto, E. Roberts-Kirchhoff, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR **288.** First-year, course-based chemistry research experience: Development and implementation of a research methods course for chemistry and biochemistry majors. **K.R. Evans**, M.J. Mio, E. Roberts-Kirchhoff

1:25 ENVR **289.** First-year, course-based chemistry research experience: Implementation of a research-based chemistry laboratory course for chemistry and biochemistry students as part of a research coordination network. **K.C. Lanigan**, A. Matti, D. Tomco, K.R. Evans

1:45 ENVR **290.** Introductory campus and distance-delivered course to engage first year undergraduates in envrionmental chemistry. **J.J. Guerard**, S.M. Hayes

2:05 ENVR **291.** Community based undergraduate research: Measurement of hazardous air pollutants with regard to environmental justice. **K. Zimmermann**, L. Young

2:25 ENVR **292.** Environmental toxicology experiments in the general chemistry laboratory curriculumat UC-Berkeley. **M.C. Douskey**, A.M. Baranger, M. Robak, L.B. Armstrong, G. Kerstiens, C.W. Tam, P. Pande

2:45 ENVR **293.** Incorporating environmental chemistry concepts into an analytical chemistry lecture/laboratory course. **D.E. Latch**

3:05 Intermission.

3:10 ENVR **294.** Can field sampling still be educationally valuable without obvious trends in the data? **S.J. Bachofer**

3:30 ENVR **295.** Analysis of heavy metals in water using cloud point extraction and flame atomic absorption spectrometry. **A. Rihana-Abdallah**, **Z. Li**

3:50 ENVR **296.** Semi-synthetic microcystins and their role in public health. **J. Westrick**, J. Birbeck, G. O'Neill

4:10 ENVR **297.** Selenium removal from power plant waters using layered double hydroxide materials. **M. Li**, L. Farmen, C.K. Chan

4:25 ENVR **298.** Real-time electronic sensor based on black phosphorus/Au NPs/DTT hybrid structure for arsenic ion detection. **G. Zhou**, J. Chen

4:40 Concluding Remarks.

Section H

San Francisco Marriott Marquis

Sierra J

Sulfidation of Metal-Based Engineered & Natural Nanomaterials: Implications for Their Fate & Effects in the Environment

P. G. Tratnyek, P. K. Westerhoff, *Organizers*

Y. Bi, D. Fan, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR **299.** Reactivity of nanoparticulate iron sulfide (mackinawite). **K.F. Hayes**

1:35 ENVR **300.** Reactivity and bioavailability of mercury sorbed to or coprecipitated with iron sulfides. N. Rivera, **H. Hsu-Kim**

2:05 ENVR **301.** Technetium stabilization in low solubility sulfide phases. M. Asmussen, **C. Pearce**, J. Neeway, A. Lawter, R. Clayton, N.P. Qafoku

2:25 ENVR **302.** Environmental application and implication of sulfide modified nanoscale zerovalent iron. **Y. Su**, A.A. Keller, X. Zhou, Y. Zhang

2:45 Intermission.

3:00 ENVR **303.** Effects of sulfidation on the reactivity of iron and iron oxides with contaminants. **P.G. Tratnyek**, D. Fan, Y. Lan, A. Agrawal

3:30 ENVR **304.** Understanding the effect of sulfidation on the reactivity of zero-valent iron materials. **W. Yan**, Y. Han

3:50 ENVR **305.** Degradation of chlorinated hydrocarbons by nanoscale zero-valent Iron treated with bisulfide and stabilized with carboxymethylcellulose. **A. Agrawal**

4:10 ENVR **306.** From the lab to the field: Development of sulfidized nanoiron for 1,2-dichloroethane degradation. **D.M. O'Carroll**, A. Nunez Garcia, C. de Boer, C. Kocur, H. Boparai, A. Chowdhury

4:40 ENVR **307.** Sulfidized nZVI particles for groundwater treatment: Synthesis, complex characterization and laboratory-scale testing. **J. Filip**, J. Slunský, J. Nosek, J. Semerád, J. Kašlík, J. Oborná, J. Bachorik, I. Medrik

Section I

San Francisco Marriott Marquis

Sierra K

Nanomaterials in Consumer Products: Formulation, Characterization & Applications Across the Product Life Cycle

S. Hussain, A. J. Kennedy, *Organizers*

C. Sayes, *Organizer, Presiding*

1:00 Introductory Remarks.

1:10 ENVR **308.** Identification and quantification of ENPs in cosmetics, food and the environment: Critical assessment of FFF-ICPMS and single-particle (multi-element) ICPMS. **F. Von Der Kammer**, A. Praetorius, M. Velimirovic, A. Gundlach-Graham, D. Günther, T. Hofmann

1:40 ENVR **309.** Development and application of methods that reliably measure graphene oxide release from aged polymer nanocomposites. **D.G. Goodwin**, D. Jacobs, L. Sung

2:00 ENVR **310.** Aging of wood stains containing CeO_2 nanoparticles as UV filters. **L. Scifo**, **A. Masion**, P. Chaurand, D. Borschneck, V. Vidal, C. Levard, J. Rose

2:20 ENVR **311.** TiO_2 nanoparticles in sunscreen lotion: Asymmetric flow field-flow fractionation hyphenated to ICPMS for their characterization. **M. Velimirovic**, S. Wagner, M. Gräf, M. Ehler, F. Abdolahpur Monikh Fazel, F. Von Der Kammer, T. Hofmann

2:40 Intermission.

2:55 ENVR **312.** Environmentally relevant physicochemical transformations of silver nanoparticles used in consumer products. **S.R. Al-Abed**, A. Gitipour, I. Radwan

3:25 ENVR **313.** Release and transformation of ZnO nanoparticles from coated surfaces during simulated dermal contact. **J.G. Clar**, E. Baumann, A. Remsen, T. Treye, T. Luxton

3:45 ENVR **314.** Determination of anions on the surface of Printed Circuit Boards (PCBs) by IPC-TM- 650 method 2.3.28 using HPIC. **B. Huang**, J. Rohrer

4:05 ENVR **315.** Influence of wear and tear on the release of silver nanoparticles from sports socks. V. Gagnon, M. Button, D. O'Carroll, **K. Weber**

4:25 ENVR **316.** *In vitro* characterization of Reactive Oxygen Species (ROS)-generating capacity of commercially available MesoSilver™ used as dietary supplement. **H. Rong**, S. Garg, T. Waite

4:45 Concluding Remarks.

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms

Sponsored by CATL, Cosponsored by COLL and ENVR

Undergraduate Research Posters

Environmental Chemistry

Sponsored by CHED, Cosponsored by ENVR and SOCED

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

S. O. Obare, *Organizer*

8:00 - 10:00

74. See previous listings.

632-634, 640-641, 645, 647, 649-650, 654, 659-666, 669-670, 675-677, 683, 687, 689-690, 710, 713, 715, 717, 720, 725, 735, 737-740, 746-747, 749, 752, 755, 758, 761-764, 770-772, 774-776, 778-780, 785, 789-790, 792, 794, 799-805, 812, 814-818, 820-821, 824-825, 829, 862, 864-865, 870, 878-882. See subsequent listings.

TUESDAY MORNING

Section A

San Francisco Marriott Marquis

Salons 10/11

ACS Award for Creative Advances in Environmental Science & Technology: Symposium in honor of Dr. Douglas R. Worsnop

Financially supported by ES&T Journal, ES&T Letters

M. Canagaratna, S. O. Obare, *Organizers*

J. L. Jimenez, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 ENVR **317.** How clusters form atmospheric aerosol particles: Nucleation in the CLOUD experiment at CERN. **U. Baltensperger**

8:35 ENVR **318.** Probing the formation, behavior, and evolution of organic particulate matter through high-resolution mass spectrometry. **N.M. Donahue**

9:00 ENVR **319.** From aerosol mass spectrometry to global models of aerosol formation. **K. Carslaw**

9:25 ENVR **320.** Highly oxidized molecules in atmospheric chemistry. **T.F. Mentel**

9:50 Intermission.

10:10 ENVR **321.** Why molecular structure matters in the chemistry of atmospheric organic aerosol formation. **P. Ziemann**

10:35 ENVR **322.** Bringing on-line aerosol and gas measurements close to home. **J.P. Abbatt**

11:00 ENVR **323.** Molecular description of SOA formation: From new particle growth rates to aqueous organic chemistry. **J. Thornton**

11:20 ENVR **324.** Chemical changes arising from the heterogeneous oxidation of atmospheric organic aerosol. **J.H. Kroll**

11:40 ENVR **325.** Atmospheric chemistry and role of isoprene hydroxy hydroperoxides: Prototype preindustrial VOC oxidation products. **F. Keutsch**

Section B

San Francisco Marriott Marquis

Salons 12/13

Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in honor of Prof. Jun Ma

Disinfection/Oxidation Byproducts Formation & Control

Financially supported by Sciex China

D. D. Dionysiou, V. K. Sharma, *Organizers*

J. Fang, *Organizer, Presiding*

S. D. Richardson, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **326.** Relative effectiveness of ferrate, chlorine dioxide, zone and peroxone for control of disinfection byproduct precursors. **D.A. Reckhow**, X. Ma, J. Bliss, J. Gao

8:30 ENVR **327.** Impacts of hydraulic fracturing on drinking water: High resolution-MS uncovers new chemical by-products of concern. **S.D. Richardson**, H.K. Liberatore, M.J. Plewa, L.H. Cizmas, J.M. Vanbriesen

8:55 ENVR **328.** Titanium dioxide and zinc oxide nanoparticles: Disinfection byproduct formation in synthetic freshwater. **L.H. Cizmas**, C. Gray, V.K. Sharma, T. McDonald

9:15 ENVR **329.** Ozone microbubbles: Mass transfer and formation of disinfection by-products. **P. Li**, Y. Yang, C. Wu, Y. Wang

9:35 ENVR **330.** Determination of trace concentrations of oxyhalides and bromide in municipal and bottled waters using a compact ion chromatography system. **J. Hu**, J. Rohrer

9:55 Intermission.

10:10 ENVR **331.** Disinfection byproducts as challenge targets for AOP treatment during potable reuse. **W. Mitch**, Y. Chuang

10:35 ENVR **332.** NDMA formation during chlorination and ozonation of N, N-dimethyl hydrazine compounds: Reaction kinetics, mechanisms, and implications for NDMA formation control. **Y. Lee**

11:00 ENVR **333.** UV/PMS disinfection: An efficient method for inactivation of four kinds of dominant fungal spores in groundwater. **G. Wen**, X. Xu, T. Huang

11:20 ENVR **334.** Enhanced bactericidal effect towards *E. coli* and removal of 1,1,1-trichloroethane by reduced graphene oxide supported FeCu. **A. Ahmad**, **X. Guo**, Y. Xu

Section C

San Francisco Marriott Marquis

Salons 14/15

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Environmental Analytical Chemistry

Cosponsored by CHED

Financially supported by AEESP

M. J. McGuire, J. A. Pedersen, *Organizers*

F. L. Rosario, *Organizer, Presiding*

8:00 ENVR **335.** Interaction of cationic pharmaceuticals with dissolved natural organic matter. **J.A. Pedersen**, I. Christl, B. Liu

8:25 ENVR **336.** Development, validation, and implications of a broad spectrum screenng method for Pharmaceuticals and Personal Care Products (PPCPs) in wastewate effluents, source waters, and finished drinking waters. **A.D. Eaton**, A. Haghani

8:50 ENVR **337.** Things you can't do with a GC-M. **S.A. Snyder**

9:15 ENVR **338.** Using dark matter accurate mass to discover NDMA precursors in wastewater. **E.M. Thurman**, I. Ferrer, D. Hanigan, P.K. Westerhoff

9:40 ENVR **339.** Polarity rapid assessment method: A promising tool for characterizing NDMA precursors in water. **C. Chen**, X. Liao, S. Li, E. Bei, J. Wang, X. Zhang

10:05 Intermission.

10:20 ENVR **340.** Analysis of water quality: A journey beyond the Abbott's building. **C.D. Hertz**

10:45 ENVR **341.** Analytical chemistry and stormwater modeling. **M.K. Stenstrom**

11:10 ENVR **342.** Understanding how hydrophobic organic pollutants distribute in urban runoff by using perylene as a probe. **M. Hsu**, I.H. Suffet

11:35 ENVR **343.** Disparate antibiotic resistance gene levels revealed across four major cities in California: A survey in drinking water, air, and soil at 24 public parks. **C.M. Echeverria Palencia**, J.A. Jay, V. Thulsiraj, N.K. Tran, C.A. Ericksen, I. Melendez, M.G. Sanchez, D. Walpert, T. Yuan, E. Ficara, N. Senthilkumar, M. Hernandez-Cira, D. Gamboa, H. Haro, S. Paulson, Y. Zhu

Section D

San Francisco Marriott Marquis

Golden Gate C1

Understanding Dissolved Organic Matter Reactivity: Honoring George Aiken, the DOM Whisperer

Y. Chin, D. M. McKnight, *Organizers*

P. Maurice, *Presiding*

8:00 Introductory Remarks.

8:10 ENVR **344.** Nanoscale metal-organic matter interactions. **H. Hsu-Kim**, C. Jiang, U. Ndu

8:45 ENVR **345.** Radium and thallium binding to dissolved organic matter. L. Martin, C. Simonucci, E. Viollier, **M.F. Benedetti**

9:10 ENVR **346.** Complexation with dissolved organic matter affects aqueous uranium speciation and adsorption. **K.M. Campbell**, C. Fuller, J. Schaper, G. Aiken

9:35 ENVR **347.** Influence of dissolved organic matter on the stability of trace level hexavalent chromium in surface and ground water samples. **V.I. Furdui**, S. Maedler

10:00 Intermission.

10:10 ENVR **348.** Can we predict metal binding by DOM? **E. Tipping**, S. Lofts, A. Stockdale

10:45 ENVR **349.** Detection of aqueous complexes of arsenic and iron with dissolved organic matter. H.V. Kulkarni, **N. Mladenov**, O. Prakash, A. Herrea

11:10 ENVR **350.** Hg-DOM interactions during removal of Hg from natural and polluted ecosystems. **F. Diaz**, L.E. Katz, D. Lawler

11:35 ENVR **351.** Photoreduction of Hg(II) and photodemethylation of methylmercury: The key role of thiol sites on dissolved organic matter. **D.E. Latch**, J.D. Jeremiason, G. Aiken, J.C. Portner, A.J. Hiranaka, M.T. Dvorak, K.T. Tran

Section E

San Francisco Marriott Marquis

Sierra A

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

D. D. Dionysiou, X. He, G. Li Puma, D. Minakata, X. Quan, *Organizers*

K. E. O'Shea, *Organizer, Presiding*

A. Sanroman, M. Valnice Boldrin Zanoni, *Presiding*

8:00 ENVR **352.** Withdrawn

8:35 ENVR **353.** Photoelectrochemical cell for simultaneous electricity generation and heavy metals recovery from wastewater. **D. Wang**, G. Li Puma

9:00 ENVR **354.** Enhanced photoelectrocatalytic degradation of organic pollutants in artificial photosynthesis systems. **L. Zeng**, **X. Li**

9:25 ENVR **355.** Enhanced filtration performance of carbon nanotube-based membrane by electrochemical assistance. **F. Xinfei**, X. Quan

9:50 Intermission.

10:05 ENVR **356.** Withdrawn.

10:40 ENVR **357.** Electrochemically enhanced microfiltration for water detoxification and fouling control in advanced wastewater treatment. **K. Choo**, H. Park, H. Park

11:05 ENVR **358.** Removal of pharmaceuticals from different waters by conventional ozonation and an electro-peroxone process. **H. Wang**, W. Yao, G. Yu, Y. Wang

11:30 ENVR **359.** Development of a novel high throughput Ti_4O_7-based reactive electrochemical filter: A case study on efficient mineralization of Perfluorooctanoate (PFOA). H. Lin, C. Wang, **J. Niu**

Section F

San Francisco Marriott Marquis

Sierra B

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Cosponsored by CEI, MEDI, ORGN and SCHB‡

Financially supported by AEESP

S. O. Obare, *Organizer*

N. Vaidya, *Organizer, Presiding*

8:30 Introductory Remarks.

8:40 ENVR **360.** Exemplifying green chemistry with sterically protected and electronically activated azamacrocycle catalysts. **R. Chorghade**, M. Chorghade

9:00 ENVR **361.** Overview of more sustainable and greener chemistry implementation in industry. **D.J. Constable**

9:40 ENVR **362.** Seamless integration of green chemistry at Pfizer from development to discovery. **D.T. Richter**

10:00 ENVR **363.** Design and evolution of the BMS process greenness scorecard. **D.K. Leahy**, E. Simmons, V. Hung, W. Fleming, J. Sweeney, M. Miller

10:20 Intermission.

10:35 ENVR **364.** Leading the textile and footwear industries towards zero discharge of hazardous chemicals: The ZDHC Foundation. **N. Sponsler**

10:55 ENVR **365.** Data and tools needed to enable toxicity-aware product-development within different industries. **N. Vaidya**

11:15 ENVR **366.** Recent green progress in the preparative and analytical separations industries. **J.P. McCauley**

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

Section G

San Francisco Marriott Marquis
Sierra C

Innovative Materials & Technologies for Sustainable Water Purification

Adsorption Technologies

Cosponsored by CEI

B. P. Chaplin, J. Choe, J. Liu, D. Shuai, W. Zhang, *Organizers*

E. L. Cates, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **367.** Measuring and modeling U(VI) adsorption to engineered iron oxide nanoparticles. **Z. Pan**, W. Li, J. Fortner, D. Giammar

8:25 ENVR **368.** Magnetic porous nanocomposites for water remediation. **K. Ventura**, R. Arrieta, V. Jabbari, D. Villagran

8:45 ENVR **369.** Removal of Cu^{2+} in aqueous system by different amine types on silica nanotube. **Y. Chun**, Y. Ko, T. Do, U. Choi

9:05 ENVR **370.** Adsorption of chlorpheniramine and N-nitrosodimethylamine formation potential toward nano-sized graphene oxide-iron oxide particle and suspension. **W. Chen**, C. Li, C. Chen

9:25 ENVR **371.** Highly efficient and specific capture of radioactive iodine in water by using gold nanoparticle-immobilized dextran gel columns. **J. Jeon**, M. Choi, H. Shim, S. Yun, S. Park, D. Choi, B. Jang

9:45 Intermission.

10:00 ENVR **372.** Innovative materials for water treatment: From custom designed adsorbents to scalable membranes. **A. Orlov**, G. Ramakrishnan, S.M. Uchimiya

10:40 ENVR **373.** Silver binding affinity of silica/melanin nanoparticles. **A.P. Zane**, M. Morgan, E. Botts, D. Olivera, J. Hoyle

11:00 ENVR **374.** Removal of hexavalent chromium from aqueous solutions by a novel biochar supported nanoscale iron sulfide composite. **Y. Gong**, H. Lyu, J. Tang

11:20 ENVR **375.** Fluorinated nanoporous networks for charged organic contaminant removal from water. J. Byun, H.A. Patel, D. Thirion, **C.T. Yavuz**

11:40 ENVR **376.** Sorption of heavy metals using tungsten oxide based sorbents. **C.K. Perkins**, T. Reed, Z. Brown, A.W. Apblett

Section H

San Francisco Marriott Marquis
Sierra J

From the Bench to the Field: Evaluating Innovative Remediation & Detection Technologies

S. R. Al-Abed, H. Henry, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **377.** Case study comparing novel remediation technologies for boron contaminated groundwater. **J.L. McKernan**, Z. Hendren, A. Vengosh, C. Northeim, S. Fang

8:25 ENVR **378.** Enhanced non-fouling membranes for water purification and recycling. **D. Battaglia**, P. Clement, J. Lange, E.P. Giannelis

8:45 ENVR **379.** Magnetic nanocomposite materials as capture agents for organic pollutants in water treatment. **A.M. Gutierrez**, T. Dziubla, J. Hilt

9:05 ENVR **380.** Bi-phase Catalyst for PCB removal from sediments and ground water. **S.M. Lomnicki**, B. Subramanian, S.R. Al-Abed, J.L. McKernan

9:25 Intermission.

9:45 ENVR **381.** Field study on the *in situ* treatment of a DNAPL source by nanoscale zero-valent iron: Effects of site oxidants. J. Ahn, C. Kim, H. Kim, K. Hwang, **I. Hwang**

10:05 ENVR **382.** Aspen Park Solvents long term cleanup of a DNAPL in fractured bedrock. **P. Stevenson**

10:25 ENVR **383.** On-site soil remediation experience in a large contaminated site by various solvents caused by illegal dumping of wastes. **K. Kawamoto**

10:45 ENVR **384.** From the bench to the field: Translating a novel plasmonic mercury sensor into a portable instrument for soils and sediments. **J. Crosby**, J. James, **D. Lucas**, C.P. Koshland

11:05 ENVR **385.** Monitoring trichloroethylene, benzene, and other VOCs in air using cavity ring-down spectroscopy and chemical dispersion. C.R. Viteri, **A.E. Miller**, M.A. Armen, B.A. Richman

11:25 ENVR **386.** Withdrawn.

Section I

San Francisco Marriott Marquis
Sierra K

Processes, Technologies & Sensors for Food-Energy-Water Nexus Research

Cosponsored by CEI and CHED

Financially supported by Electric Power Research Institute (EPRI), National Science Foundation (NSF)

W. J. Cooper, *Organizer*

S. Bushart, N. S. Rao, *Organizers*, *Presiding*

W. Cooper, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **387.** Intensive aquatic protein production using duckweed as a model platform. **A. McQuilling**, J. Lawson, S. Mukhtar, W. Grieco

8:25 ENVR **388.** Vibration-driven droplet motion on a flapping film for water collection. **M. Derby**, R. Huber, N. Doughramaji, X. Chen

8:45 ENVR **389.** Redox-based electrochemical technologies for energy-efficient water purification and wastewater treatment. **X. Su**, T.F. Jamison, T. Hatton

9:05 ENVR **390.** Highly permeable thin film composite membranes with nanocomposite barrier layer for desalination applications. K. Liu, H. Ma, **B.S. Hsiao**

9:25 ENVR **391.** Capacitive nutrient removal and recovery from anaerobic membrane bioreactor effluent. **Z. Ge**, **Z. Ren**

9:45 Intermission.

10:00 ENVR **392.** Olefin/paraffin separation properties of graphene oxide membranes. **B. Yoo**, S. Lee, H. Park

10:20 ENVR **393.** Toward energy-neutral and decentralized water re-use with flow-electrode capacitive deionization. **K. Hatzell**, **M. Hatzell**, M. Dixit, D. Moreno

10:40 ENVR **394.** Characterization and implications of cometabolic bio-methanol production by ammonia oxidizing bacteria. **Y. Su**, L. Arellano-García, S. Sathyamoorthy, K. Chandran

11:00 ENVR **395.** Carbon nanotube enabled water treatment. **S. Ragunath**, S. Roy, S. Mitra

11:20 ENVR **396.** Algae cultivation on a pilot-scale Algal Turf Scrubber® from dairy wastewater for bioremediation and sustainable biofuel production. **J. Yan**

11:40 Concluding Remarks.

Mineral-Water Interface Chemistry

Sponsored by GEOC, Cosponsored by COLL and ENVR

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Sponsored by CATL, Cosponsored by ENVR and I&EC

Elucidation of Mechanisms & Kinetics on Surfaces

Electrons

Sponsored by CATL, Cosponsored by COLL and ENVR

TUESDAY AFTERNOON

Section A

San Francisco Marriott Marquis
Salons 10/11

ACS Award for Creative Advances in Environmental Science & Technology: Symposium in honor of Dr. Douglas R. Worsnop

Financially supported by ES&T Journal, ES&T Letters

J. L. Jimenez, S. O. Obare, *Organizers*

M. Canagaratna, *Organizer, Presiding*

1:30 ENVR **397.** Recent advances in atmospheric chemistry studies: Applications of mass spectrometric methods. **J.T. Jayne**

1:50 ENVR **398.** Dielectric spectroscopy and glass transitions of organic molecules and mixtures prepared from submicron particle deposition. **P. Davidovits**

2:10 ENVR **399.** Toward understanding aqueous-phase chemistry of secondary organic aerosol via aerosol mass spectrometry. **Q. Zhang**

2:30 ENVR **400.** Aerosol mass spectrometry of refractory black carbon particles: Black carbon particles in the atmosphere. **T.B. Onasch**

2:50 ENVR **401.** Aerosol composition and properties in the developing world. **H. Coe**

3:10 Intermission.

3:25 ENVR **402.** Bright future of the potential aerosol mass concept and chamber. **W. Brune**

3:50 ENVR **403.** Recent results on organic aerosol sources and properties, and on the experimental systems used to study them. **J. Jimenez**

4:15 ENVR **404. Award Address** (ACS Award for Creative Advances in Environmental Science & Technology sponsored by the ACS Division of Environmental Chemistry & the ACS Publications Journals Environmental Science & Technology & Environmental Science & Technology Letters). Mass spectrometry of atmospheric aerosol: 1 nanometer to 1 micron. **D.R. Worsnop**

Section B

San Francisco Marriott Marquis
Salons 12/13

Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in honor of Prof. Jun Ma

Membrane & Adsorption Technologies

Financially supported by Sciex China

D. D. Dionysiou, J. Fang, V. K. Sharma, *Organizers*

S. Lin, L. Tang, *Presiding*

1:30 Introductory Remarks.

1:35 ENVR **405.** Membrane fouling bevavior of composite coagulant PAC-PDMDAAC under different membrane materials in coagulation-ultrafiltration combined process. X. Shen, **B. Gao**, Q. Yue

2:00 ENVR **406.** Anti-oil-fouling membranes in membrane distillation: Drivers, materials development, and force spectroscopy for mechanisms elucidation. **S. Lin**, Z. Wang

2:25 ENVR **407.** Bioinspired polydopamine and silver nanoparticles form *in situ* on membrane surface to mitigate biofouling. **L. Tang**, K.J. Livi, K. Chen

2:45 ENVR **408.** Preparation and properties of PVDF adsorption membrane. **Y. Zhang**

3:05 ENVR **409.** Development of nanocomposite membrane process for drinking water treatment. **P. Wang**, D. Song, Z. Sun, L. Ru, H. Wang, F. Wang, H. Jiang, J. Ma

3:25 Intermission.

3:40 ENVR **410.** Enhanced removal of trace antimony(V) in water by iron oxide supported by chitosan/cellulose acetate. **J. Yang**, H. Chen, Z. Li, R. Bai

4:05 ENVR **411.** Adsorption behavior of Cu(II) ions from aqueous medium on TEMPO-mediated oxidized cellulose nanofibers. **P. Liu**, A. Mathew, H. Sehaqui

4:25 ENVR **412.** Adsorption of Cs in water using functionalized, templated and magnetic mesoporous composites. **K. Guo**, F.X. Han, Z. Arslan, R. Zhang, Y. Zhang, C. Rogers

4:45 ENVR **413.** Ammonia nitrogen adsorption onto modified zeolites at low temperature. **L. Qiu**, Q. Qiu, L. Zhu, S. Zhang

5:05 ENVR **414.** Critical effect of solute species and concentrations on cation exchange behavior of thin-film composite membranes in forward osmosis. **X. Lu**, W. Cheng, Y. Yang, J. Ma

Section C

San Francisco Marriott Marquis
Salons 14/15

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

Source Water Quality

Cosponsored by CHED

Financially supported by AEESP

J. A. Pedersen, F. L. Rosario, *Organizers*

M. J. McGuire, *Organizer, Presiding*

1:30 ENVR **415.** Wildfires: Burning questions regarding drinking water supplies and treatment. **A.D. Revchuk**, I.H. Suffet

1:55 ENVR **416.** Laboratory simulation of wildfire heating: Effects on DOM and water treatment. **A.K. Hohner**, F.L. Rosario

2:20 ENVR **417.** Effect of fire-impacted source water on ozonation kinetics in drinking water treatment. **Z. Wu**, M. Mizel, T.M. Young

2:45 ENVR **418.** Mobilization of nitrogenous pyrogenic soil organic matter in wildfire-affected watersheds and its impact on the formation of haloacetonitriles. **Y. Yu**, F.L. Rosario

3:10 Intermission.

3:25 ENVR **419.** Evaluation of prevailing flush guidelines to reduce water lead exposures: Implications for regulations and public health outreach. **A.L. Katner**, K. Pieper, J. Parks, K. Brown, C. Hu, H. Lin, X. Wang, J. Diaz, M. Edwards

3:50 ENVR **420.** Barriers to access to chemical data for source water vulnerability assessments. **J. Rosen**

4:15 ENVR **421.** Mexico City: The case for integrative science and policy. **T.J. Downs**

4:40 ENVR **422.** Federal framework for regulating acidization, a sister-technology to hydraulic fracturing. **K. Abdullah**, I.H. Suffet, M. Stenstrom, T. Malloy

Section D

San Francisco Marriott Marquis
Golden Gate C1

Understanding Dissolved Organic Matter Reactivity: Honoring George Aiken, the DOM Whisperer

Y. Chin, D. M. McKnight, *Organizers*

E. J. O'Loughlin, *Presiding*

1:30 ENVR **423.** Comparison of the properties of different natural organic matter samples from the Suwannee River (GA, USA). **P. Maurice**

2:05 ENVR **424.** Effects of dissolved organic matter on the fate and transformation of nanosized zero-valent iron in aqueous system. **C. Kim**, Y. Chin, J. Ahn, M.L. Wei-Haas, B. McAdams, I. Hwang

2:30 ENVR **425.** Impact of Natural Organic Matter (NOM) on the formation and reactivity of iron oxide particles formed on Fe(III) and Fe(II) addition: Comparison of terrigenous NOM versus Algogenic NOM. **S. Garg**, K. Wang, D. Waite

2:55 ENVR **426.** Dark formation of hydrogen peroxide upon oxidation of dissolved organic matter. **C. Chu**, N. Walpen, M. Sander, K.P. McNeill

3:20 Intermission.

3:30 ENVR **427.** Exploring the relationships between the redox and mineral adsorption properties of DOM. **B. McAdams**, G. Aiken, J. Hudson, **Y. Chin**

4:05 ENVR **428.** Dissolved organic matter-mediated solar degradation of endocrine-disrupting pollutants in natural waters. **J. Gray**, D.E. Latch, K. Daumit, G. Aiken

4:30 ENVR **429.** Understanding DOM-organic contaminant attenuation of non-polar organic pollutants. **M. Hsu**, I.H. Suffet

4:55 ENVR **430.** Effect of NOM and water hardness on Diffusive Gradient in Thin-Film (DGT) prediction of bioaccumulation by yellow lampmussel and fathead minnow. **G.L. Mills**, R. Philipps, R. Bringoff

5:20 Concluding Remarks.

Section E

San Francisco Marriott Marquis
Sierra A

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

X. He, G. Li Puma, D. Minakata, K. E. O'Shea, X. Quan, *Organizers*

D. D. Dionysiou, *Organizer, Presiding*

D. Hermosilla, *Presiding*

1:30 ENVR **431.** 1,4-dioxane treatment by advanced oxidation processes: Current situation, future perspectives, and potential industrial implementation. **D. Hermosilla**, H. Barndök, N. Merayo, A. Blanco

2:05 ENVR **432.** Withdrawn.

2:30 ENVR **433.** TiO_2 Photocatalytic degradation of the flame retardant, tris (2-chloroethyl) phosphate: Kinetic and mechanistic studies. **A. Abdullah**, K.E. O'Shea

2:55 ENVR **434.** Kinetic modeling of sunlight-assisted degradation of trace organic substances. **H. Vo**

3:20 Intermission.

3:35 ENVR **435.** Withdrawn

4:00 ENVR **436.** Color-stripping of dye-containing wastewater by a new H_2O_2/Cu(II)-phenanthroline AOP. **E. Walger**, F. Molton, C. Duboc, N. Marlin, G. Mortha

4:25 ENVR **437.** Withdrawn

4:50 ENVR **438.** Is it time to replace traditional UV lamps by UV-Light Emitting Diodes (UVLEDs) in water treatment industry? Towards sustainable photovoltaic-powered UVLED photoreactors. **M. Eskandarian**

Section F

San Francisco Marriott Marquis
Sierra B

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Cosponsored by CEI, MEDI, ORGN and SCHB‡

Financially supported by AEESP

S. O. Obare, *Organizer*

N. Vaidya, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **439.** Sustainable applications of magnetic nano-catalysts and graphitic carbon nitrides. **R.S. Varma**

1:55 ENVR **440.** Advancing greener reptide and oligonucleotide syntheses. **M.E. Kopach**

2:15 ENVR **441.** Chemetry's Shuttle™ process: New technology platform to produce caustic soda and EDC while eliminating chlorine gas and saving energy. **M.K. Leclerc**

2:35 ENVR **442.** Green process development using chiral resolution. **N.A. Vaidya**

2:55 ENVR **443.** Evolution of chiral HPLC toward greener techniques. **R. Romero**

3:15 Intermission.

3:30 ENVR **444.** Biologics: The new frontier for green chemistry in the pharma industry. **K. Budzinski**, D. O'Connor

3:50 ENVR **445.** Key consideration when choosing a manufacturing solvent in pharmaceutical manufacturing. **A. Mehta**

4:10 Panel Discussion.

Section G

San Francisco Marriott Marquis
Sierra C

Innovative Materials & Technologies for Sustainable Water Purification

Adsorption Technologies

Cosponsored by CEI

E. L. Cates, J. Choe, J. Liu, D. Shuai, W. Zhang, *Organizers*

B. P. Chaplin, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **446.** Hemoglobin/iron oxide composite: Synthesis, characterization and adsorption of organic dyes. **M. Essandoh**, R.A. Garcia

1:55 ENVR **447.** Cationic materials for reversible, selective perchlorate trapping. **S. Oliver**

2:15 ENVR **448.** Selective silica separations from waste water using ion-exchange media. **K. Sasan**, T.M. Nenoff, P.V. Brady, J. Krumhansl

2:35 ENVR **449.** Withdrawn.

2:55 Intermission.

3:10 ENVR **450.** Removal of oxyanion pollutants from water by bicomponent metal oxide adsorbents. **Y. Zou**, Y. Wang

3:30 ENVR **451.** Removal of heavy metals from drinking water using hydrothermal char. **M.T. Timko**

3:50 ENVR **452.** Rapid removal of phosphate from wastewater using magnetized fast pyrolysis biochar from waste Douglas fir. **A.G. Karunanayake**, M. Crowley, R. Anderson, T.E. MIsna

4:10 ENVR **453.** Withdrawn.

4:30 ENVR **454.** Removal of perfluoroalkyl substances from water using molecularly engineered coatings on sand and silica. **P. Edmiston**

4:50 ENVR **455.** Arsenic, cadmium, nickel and lead adsorption mechanism, kinetics and thermodynamics of copper based and iron based metal organic framework. **A. Yurdusen**, Y. Yurum

Section H

San Francisco Marriott Marquis
Sierra J

From the Bench to the Field: Evaluating Innovative Remediation & Detection Technologies

S. R. Al-Abed, H. Henry, *Organizers*, *Presiding*

1:30 ENVR **456.** Unexpected ring cleavage products from $OH^•$ and $SO_4^{•-}$ treatment of contaminants. **J. Van Buren**, C. Prasse, B. Skeel, D.L. Sedlak

1:50 ENVR **457.** Mechanisms on the impacts of alkalinity, pH and chloride on heterogeneous persulfate activation for groundwater remediation. **W. Li**, H. Liu

2:10 ENVR **458.** Enhanced bioremediation of PAH contaminated soils: Combining novel molecular techniques with targeted bioaugmentation strategies. **L. Redfern**, C.K. Gunsch

2:30 ENVR **459.** Investigating polychlorinated biphenyl biodegradation potential in contaminated sediments with chemical and molecular biology approaches. Y. Liang, A. Martinez, J. Ewald, A. Awad, J.L. Schnoor, **T. Mattes**

2:50 Intermission.

3:10 ENVR **460.** Metagenomic analysis of mobile elements and phage in Trichloroethene (TCE) dechlorinating communities. **R. Keren**, V. Brisson, M. Xinwei, M. Yujie, K. Yu, J.F. Banfield, L. Alvarez-Cohen

3:30 ENVR **461.** Probing active acidophilic methanotrophs involved in chlorinated solvent biodegradation. **Y. Shao**, K. Chu

3:50 ENVR **462.** Bioprocess development for 1,4-dioxane treatment: Bench through field investigation. F. Shirazi, **A. Razavi**, A. Gregg, C. McGrath, N. Hlavacek, J. Salanitro

4:10 ENVR **463.** Biomarkers for validating natural and enhanced biodegradation of 1,4-dioxane in groundwater. P. Gedalanga, Y. Miao, A. Madison, T. Richards, W. Gierke, H. Holbrook, R. Mora, D. Chiang, **S. Mahendra**

4:30 ENVR **464.** From infancy to full-scale demonstration: The twenty year development of electrokinetically-enhanced bioremediation for successful treatment of chlorinated solvents in clays and silts. **N.D. Durant**, J. Wang, E. Cox, D. Gent

Section I

San Francisco Marriott Marquis
Sierra K

Science & Perception of Climate Change

Cosponsored by CEI and CHED

Financially supported by AEESP

S. O. Obare, *Organizer*

E. Schoffers, *Organizer, Presiding*

1:30 ENVR **465.** How culture shapes the climate change debate. **A.J. Hoffman**

2:10 ENVR **466.** Climate science literacy: An imperative for the next generation. **G.P. Foy**

2:40 ENVR **467.** Facing the new world of climate disruption. **J.A. Bell**

3:00 ENVR **468.** Visualizing and understanding the science of climate change. **P.G. Mahaffy**

3:30 ENVR **469.** Why do students respond favorably to attempts to teach climate change? **G.M. Bodner**

‡ *Cooperative Cosponsorship*

3:55 ENVR **470.** Does science get lost in translation? How popular media frames the climate change debate. **E. Schoffers**

4:15 ENVR **471.** Educating communities about the impact of climate change. **C.M. Crudden**

4:35 ENVR **472.** ACS action needed to influence attitudes and behavior on climate change. **B.Z. Shakhashiri**

5:00 Panel Discussion.

Mineral-Water Interface Chemistry

Sponsored by GEOC, Cosponsored by COLL and ENVR

Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce

Sponsored by CHAL, Cosponsored by CHAS, ENVR and I&EC

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Sponsored by CATL, Cosponsored by ENVR and I&EC

Elucidation of Mechanisms & Kinetics on Surfaces

Organic Oxygenates

Sponsored by CATL, Cosponsored by COLL and ENVR

WEDNESDAY MORNING

Section A

San Francisco Marriott Marquis
Salons 10/11

Great Achievements in Environmental Science & Technology: James J. Morgan Award Symposium

Financially supported by ES&T Journal, ES&T Letters

A. Grostern, *Organizer*

D. Sedlak, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ENVR **473.** Biological and chemical activities of extracts from plastics collected from the North Pacific Gyre and plastics treated with UV-light. **D. Schlenk**, S.L. Coffin, J. Gan

8:30 ENVR **474.** Explaining the presence of respiratory tract opportunistic bacterial pathogens in drinking water systems. **L. Raskin**, S. Haig, N. Kotlarz, J. LiPuma

8:55 ENVR **475.** Stable isotope view of the formation of *N*-nitrosodimethylamine during water disinfection with chloramine. **T.B. Hofstetter**, S. Spahr, U. von Gunten

9:20 ENVR **476.** Is bioremediation of PAH contaminated soil worth it? **S. Simonich**

9:45 ENVR **477.** Photochemical conversions at the interfaces of semiconductor hybrids for environmental applications. **W. Choi**

10:10 Intermission.

10:25 ENVR **478.** Impacts of the Minamata Convention on mercury in Asia. **N. Selin**, A. Giang, L.C. Stokes, E.S. Corbitt, D.G. Streets, V.J. Karplus, D. Zhang, K.M. Mulvaney, M. Li, C. Li, S.Y. Kwon

10:50 ENVR **479.** Investigation into the transfer of biological species from the ocean to the atmosphere: Mother nature's way of controlling climate? **K.A. Prather**, C. Gaston

11:15 ENVR **480.** Working on environmental challenges as an engineer gone wrong. **M.S. Mauter**

11:45 Concluding Remarks.

Section B

San Francisco Marriott Marquis
Salons 12/13

Oxidation Processes, Nanoparticles & Membranes in Water & Wastewater Treatment: A Symposium in honor of Prof. Jun Ma

Nanoparticles & Nanomaterials

Financially supported by Sciex China

J. Fang, *Organizer*

D. D. Dionysiou, V. K. Sharma, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **481.** Nanostructured eco-materials based on clay minerals: Synthesis and applications in organic contaminants transformation and heavy metal removal. **C. Wang**

8:30 ENVR **482.** Application of natural organic matter coated magnetic iron oxide nanoparticles for the remediation of arsenic and selenium. **M. Rashid**, Y. Cai, G. Sterbinsky, K.E. O'Shea

8:50 ENVR **483.** Withdrawn.

9:10 ENVR **484.** Nanoparticles removed by $AlCl_3$ in the process of coagulation. **L. Zhang**

9:30 ENVR **485.** Advances of nano-sized metal oxides formed *in situ* for the enhanced coagulation of surface water and removal of heavy metals, algae. **L. Wang**, Y. Liu, J. Ma

9:50 Intermission.

10:05 ENVR **486.** Synthesis of novel carbon spheres and their supported Fe nanoparticles for removal of metronidazole. **X. Wang**

10:25 ENVR **487.** N-doped carbon nanotubes for advanced oxidation processes. R.R. Rocha, O. Soares, A. Gonçalves, J. Órfão, J. Figueiredo, **M.R. Pereira**

10:45 ENVR **488.** Catalytic effects of carbon nanomaterials in abiotic transformation of organic contaminants: Implications for water and wastewater treatments. **W. Chen**, L. Duan, C. Zhang, M.B. Tomson, P.J. Alvarez

11:05 ENVR **489.** Development and application of layered carbon materials in advanced oxidation processes for water purification. **F. Qi**, B. Xu, Z. Song

11:25 ENVR **490.** Investigations on oxidation processes, nanoparticles, and membranes in water and wastewater treatment with engineering applications. **J. Ma**, J. Jiang, P. Wang, Y. Zhou, Y. Gao, H. Cheng, X. Liu, D. Song

Section C

San Francisco Marriott Marquis
Salons 14/15

Chemical Principles of Environmental, Cellular & Organismal Nanotoxicology

Cosponsored by COLL

C. Celle, L. L. Charlet, J. Simonato, C. Vulpe, *Organizers*

B. Gilbert, S. Lehman, *Organizers*, *Presiding*

D. Arndt, *Presiding*

8:00 ENVR **491.** Contribution of phagolysosomal membrane permeability to micro and nanoparticle toxicity. **A. Holian**

8:30 ENVR **492.** Structure activity relationships of engineered nanomaterials in inducing NLRP3 inflammasome activation and chronic lung fibrosis. **T. Xia**

9:00 ENVR **493.** Imogolite nanotubes as model HARN: Synthesis strategies and toxicological assesment. A. Masion, C. Levard, E. Doelsch, **A. Avellan**, C. Mauroy, W. Liu, J. Rose, C. Santaella, W. Achouak

9:20 ENVR **494.** Impact of silver nanowire length and diameter on rainbow trout RTgillW1 and RTgutGC cell lines. **D. Arndt**, D. Toybou, J. Simonato, C. Celle, B. Gilbert, L.L. Charlet, C. Vulpe, S. Lehmann

9:40 ENVR **495.** Toward safer silver nanowires by design: Modulation of characteristics and evaluation of dermal toxicity. **S. Lehmann**, B. Gilbert, M. Viau, D. Toybou, J. Simonato, C. Celle, T. Maffeis, L.L. Charlet

10:00 Intermission.

10:20 ENVR **496.** Spectroscopic insights into the role of defects in nano-bio interactions. **R. Podila**, J. Brown

10:50 ENVR **497.** Identifying the molecular mechanisms responsible for differences in toxicity of complex nanomaterials across organisms. **R. Klaper**, J. Bozich, J. Crago, B. Curtis, V. Feng, M. Hang, R.J. Hamers, C.L. Haynes, E. Melby, C.J. Murphy, N. Niemuth, G. Orr, T.A. Qiu, K. Zhang

11:10 ENVR **498.** Biological Impact of nanoscale lithium-intercalating battery materials to model bacterium *Bacillus subtilis*. **V. Feng**, M. Hang, T. Linn, B. Miller, R.J. Hamers

11:30 ENVR **499.** Integrated chemical and toxicological investigation of fullerene after UV/UV-chlorine drinking water treatment. **C. Zhang**, Q. Zhang

Section D

San Francisco Marriott Marquis
Golden Gate C1

Novel Membrane Materials & Processes for Water Purification

D. Jassby, B. Mi, *Organizers*, *Presiding*

8:00 ENVR **500.** Artificial water channel based membranes. **M. Kumar**, Y. Shen, T. Ren

8:30 ENVR **501.** Artificial water channels exhibiting enhanced dipolar water translocation. **M.D. Barboiu**

8:50 ENVR **502.** Two-dimensional MoS_2 nanosheets: An emerging material for advanced water separation membranes. **Z. Wang**, S. Zheng, J. Urban, B. Mi

9:10 ENVR **503.** Covalent organic frameworks as novel membrane materials. **L. Valentino**, M. Matsumoto, W.R. Dichtel, M. Abdulsalam, A. Livingston, B.J. Marinas

9:30 ENVR **504.** Polycrystalline metal-organic framework membranes for water purification. **D. Zhao**, X. Wang

9:50 Intermission.

10:10 ENVR **505.** Development of polymer-graphene oxide based filter coatings for simultaneous removal of heavy metals, nitrate and microorganisms. **D.F. Rodrigues**, P. Bandara, E.T. Nadres

10:40 ENVR **506.** Understanding graphene oxide swelling properties in aqueous phase. **S. Zheng**, J. Urban, Q. Tu, S. Li, B. Mi

11:00 ENVR **507.** Breathable graphene oxide toxicant barriers. **R. Spitz**, M. Cruz, N. Mahfouz, Y. Qiu, R. Hurt

11:20 ENVR **508.** Co-assembly of graphene oxide and magnetic bimetallic nanoparticle for highly efficient removal of tetracycline. **P. Tabrizian**, S. Rahaman

Section E

San Francisco Marriott Marquis
Sierra A

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

D. D. Dionysiou, X. He, G. Li Puma, K. E. O'Shea, X. Quan, *Organizers*

D. Minakata, *Organizer, Presiding*

N. H. Ince, *Presiding*

8:00 ENVR **509.** Single, simultaneous and sequential applications of ultrasonic frequencies to eliminate pharmaceutical residues in water. **N.H. Ince**, A. Ziylan Yavas

8:35 ENVR **510.** Kinetic, product, and computational studies of the ultrasonically induced degradation of 4-methylcyclohexanemethanol (MCHM). **D. Cui**, A.M. Mebel, L.E. Arroyo-Mora, H. Holness, K. Furton, K.E. O'Shea

9:00 ENVR **511.** High performance Magnéli phase reactive electrochemical membranes for oxidation and reduction of water contaminants. **B.P. Chaplin**, S. Nayak

9:25 ENVR **512.** Co-effects of UV/H_2O_2 and natural organic matter on the surface properties and colloidal stability of cerium oxide nanoparticles. **X. Wu**, C.W. Neil, H. Jung, Y. Jun

9:50 Intermission.

10:00 ENVR **513.** Abatement of polychoro-1,3-butadienes in aqueous solution by ozone, UV-photolysis, and advanced oxidation processes (O_3/H_2O_2 and UV/H_2O_2). **M. Lee**, T. Merle, D. Rentsch, S. Canonica, U. von Gunten

10:25 ENVR **514.** Treatment of 11-nor-9-carboxy-Δ^9-tetrahydrocannabinol (THC-COOH) through advanced oxidation processes. Y. Park, A. Mackie, **G. Gagnon**

10:50 ENVR **515.** Withdrawn.

11:15 ENVR **516.** Use of multivariable analysis (anova) to compare irradiation sources on diuron destruction by photocatalysis using TiO_2-P25 Impregnated with Sm^{3+}, Eu^{3+} and Gd^{3+}. J. Torres Torres, **J. Arevalo Perez**, H. Perez Vidal, I. Cuauhtemoc Lopez

11:40 ENVR **517.** Treatment of emerging contaminants by UV/H_2O_2 in water detoxification & reuse applications. Y. Huang, Y. Liu, W. Abdelraheem, K.H. Cochran, E.G. Xu, S.D. Richardson, D. Schlenk, **D.D. Dionysiou**

Section F

San Francisco Marriott Marquis

Sierra B

Aquatic Photochemistry

Cosponsored by GEOC

Financially supported by AEESP

W. Arnold, V. Lin, *Organizers*

K. P. McNeill, *Organizer, Presiding*

8:30 ENVR **518.** Identification and toxicity testing of the photochemical degradation products of octyl methoxycinnamate, a common organic UV filter chemical. C. Berg, H. Stein, J. Maung, L. O'Connor, A. Pagano, M.G. Paulick, **L. MacManus-Spencer**

8:50 ENVR **519.** Photochemical fate of lampricides in tributaries of the Great Lakes. **C.K. Remucal**, M. McConville, A. Ward

9:10 ENVR **520.** Effect of agricultural dissolved organic matter on the photolytic fate of poultry antibiotics. **K. Mangalgiri**, L.M. Blaney

9:30 ENVR **521.** p-Nitroanisole/pyridine and p-nitroacetophenone/pyridine actinometers revisited: Quantum yield corrections based on ferrioxalate. J.R. Laszakovits, S. Berg, J. O'Brien, K.H. Wammer, **C.M. Sharpless**

9:50 ENVR **522.** Singlet oxygenation of dienes in water and methanol: Domoic acid, sorbate, and sorbic alcohol. **M. Jaramillo**, K.E. O'Shea

10:10 Intermission.

10:20 ENVR **523.** Photomineralization of 5-halogenosalicylic acids: A self-sustained reaction via the formation of Light Induced Secondary OH precursors (LIS-OH). R. Tafer, **M. Sleiman**, P. De sainte claire, P. Vicendo, A. Boulkamh, C. Richard

10:40 ENVR **524.** Compound specific isotope analysis of aqueous photodegradation of substituted chlorobenzenes. **E. Passeport**, N. Zhang, L. Wu, H. Herrmann, B. Sherwood Lollar, H. Richnow

11:00 ENVR **525.** QSARs for phenols and phenolates: Oxidation potential as a predictor of reaction rate constants with photochemically produced oxidants. **W. Arnold**, Y. Oueis, M. O'Connor, J. Rinaman, M. Taggart, R. McCarthy, K. Foster, D.E. Latch

11:20 ENVR **526.** Chemically accurate aqueous redox potentials for organic pollutants via high-speed cyclic voltammetry and Molecular Dynamics (MD)/Equation-of-Motion Coupled Cluster (IP-EOM-CCSD) simulations. M. Paul, D. Ruuska, **S.N. Eustis**

11:40 ENVR **527.** Use of 4-(dimethylamino) benzonitrile to probe the photosensitizing and inhibitory effects of dissolved organic matter. **S. Canonica**, F. Leresche, L. Ludvíková, D. Heger, P. Klan, U. von Gunten

Section G

San Francisco Marriott Marquis

Sierra C

Innovative Materials & Technologies for Sustainable Water Purification

Membrane & Other Treatment

Cosponsored by CEI

E. L. Cates, B. P. Chaplin, J. Liu, D. Shuai, W. Zhang, *Organizers*

J. Choe, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENVR **528.** Pseudocapacitive deionization: Desalination of water using high capacity MnO_2 electrodes. **S. Hand**, R. Cusick

8:55 ENVR **529.** Molecular insight of ethinylestradiol (EE2) interaction with polymer membranes in waste water purification. **C.D. Domilongo Bope**, A. Nalaparaju, N.K. Chun, Y. Cheng, B. Cao, L. Lu

9:15 ENVR **530.** Effect of pre-ozonation and membrane modification with carbon nanotubes on fouling control. **J. Guo**

9:35 ENVR **531.** Porous CNT Joule heaters in ionizable environments and their use in desalination: Frequency dependent stability and application in MD. **A.V. Dudchenko**, C. Chen, A. Cardenas, J. Rolf, D. Jassby

9:55 Intermission.

10:10 ENVR **532.** Next generation of water purification membranes made of 2D nanomaterials: Promises and challenges. **B. Mi**, S. Zheng, Z. Wang, C. Finnerty

10:50 ENVR **533.** Toward a multi-layered multi-functional filter: Using cellulose acetate electrospun nanofibers and renewable nanomaterials for water purification. **C. Fausey**, J.B. Zimmerman

11:10 ENVR **534.** Nanoscale zero-valent iron in mesoporous carbon (nZVI@C): Stable nanoparticles for precious metal extraction. **W. Teng**, J. Fan, W. Zhang, D. Zhao

11:30 ENVR **535.** Preventing regrowth of nitrosamines during wastewater reuse by manipulating chloramine chemistry. **D. McCurry**

Section H

San Francisco Marriott Marquis

Sierra J

Poly- & Per-Fluoroalkyl Substances: Where, What, When, Why, Who & How

K. Chu, L. S. Lee, J. Liu, V. Yingling, *Organizers*, *Presiding*

8:00 ENVR **536.** Perfluoroalkyl ether carboxylic acids: Occurrence in the Cape Fear river watershed and fate in drinking water treatment processes. **D. Knappe**, M. Sun, L. Dudley, E. Arevalo, M. Strynar, A. Lindstrom

8:25 ENVR **537.** Minnesota Poly- and Perfluoroalkyl Substance (PFAS) megaplume: A case study of PFAS fate and transport and implications for site investigation and drinking water treatment. **V. Yingling**

8:50 ENVR **538.** Poly- and perfluoroalkyl substances in soil following aqueous film forming foam deployment during firefighting efforts after the train derailment in Lac-Mégantic, Québec. **S. Mejia- Avendaño**, G. Munoz, S. Vo Duy, M. Desrosiers, S. Sauvé, J. Liu

9:15 ENVR **539.** Estimating the number PFAS contaminated airports in Canada. S. Milley, P. Fortin, N. Battye, D. Loock, I. Koch, D. Reynolds, **K. Weber**

9:40 Intermission.

10:10 ENVR **540.** Biodegradability of Polyfluoroalkyl Phosphates (PAPs), fluorotelomer alcohol-based surfactants. M. Lewis, M. Kim, N. Wang, **K. Chu**

10:35 ENVR **541.** Isomer-Specific biotransformation of N-Ethyl Perfluorooctane Sulfonamide Ethanol (EtFOSE) in aerobic soil. **J. Liu**, G. Zhong, W. Li, S. Mejia Avendaño

11:00 ENVR **542.** Sorption of Poly- and Perfluoroalkyl Substances (PFASs) relevant to Aqueous Film Forming Foam (AFFF)-impacted groundwater by biochars and activated carbon. X. Xiao, B. Ulrich, B. Chen, **C.P. Higgins**

11:25 ENVR **543.** Fate and transport modeling of co-occurring PFOS, MTBE, and BTEX in a fractured chalk aquifer. **I. Ross**, J. Burdick, J. McDonough, J. Miles, J. Hurst, E. Houtz

11:50 Concluding Remarks.

Section I

San Francisco Marriott Marquis

Sierra K

Whole Organism Metrology to Support Nanotoxicology Research in the Environment

S. K. Hanna, C. M. Sims, *Organizers*

M. Johnson, B. C. Nelson, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 ENVR **544.** Agglomeration of *Escherichia coli* with positively charged nanoparticles can lead to artifacts in a standard *Caenorhabditis elegans* toxicity assay. **S.K. Hanna**, A.R. Montoro Bustos, A.W. Peterson, V. Reipa, L.D. Scanlan, S. Hosbas Coskun, T. Cho, M. Johnson, V.A. Hackley, B.C. Nelson, M.R. Winchester, J.T. Elliott, E. Petersen

9:00 ENVR **545.** High-throughput single-cell ICP-MS methods development and application to study algaecide and nanoparticles interaction and toxicity to unicellular organism cyanobacteria. **H. Shi**, K. Li, H. Zhang, H. Jiang, C. Stephan

9:25 ENVR **546.** Separation, sizing, and quantitation of engineered nanoparticles in an organism model using inductively coupled plasma mass spectrometry and image analysis. **M. Johnson**, S.K. Hanna, A.R. Montoro Bustos, C.M. Sims, L. Elliott, A. Lingayat, A.C. Johnston, B. Nikoobakht, J.T. Elliott, D. Holbrook, K.C. Scott, K. Murphy, E. Petersen, L. Yu, B.C. Nelson

9:50 Intermission.

10:05 ENVR **547.** Single cell and single particle ICP-MS analysis of nanohybrids. **J. Lead**

10:30 ENVR **548.** Systems-level approach to characterizing effects of ENMs in terrestrial organisms and ecosystems. **C.M. Rico**, M.G. Johnson, J.R. Reichman, C.P. Andersen

10:55 ENVR **549.** Nanoparticle uptake in plant cells: A nano-CT and hyperspectral imaging study. **A. Masion**, A. Avellan, C. Levard, F. Schwab, D. Borschneck, C. Perrine, C. Santaella

11:20 ENVR **550.** Novel image and data fusion method to improve spatial resolution and spectral content of biological images using ToF-SIMS. **T.M. Milillo**, R. Fischione, A. Montes, J.A. Gardella

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

Sponsored by GEOC, Cosponsored by COLL, ENVR and NUCL

Mineral-Water Interface Chemistry

Sponsored by GEOC, Cosponsored by COLL and ENVR

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Fundamental Structure-Activity Relationships: The Interface of Operando with Physical Sciences

Sponsored by CATL, Cosponsored by ENVR and I&EC

Elucidation of Mechanisms & Kinetics on Surfaces

Organic Oxygenates

Sponsored by CATL, Cosponsored by COLL and ENVR

WEDNESDAY AFTERNOON

Section A

San Francisco Marriott Marquis

Salons 10/11

Pesticides in Surface Water: Monitoring, Modeling, Mitigation, Risk Assessment & Regulation

Financially supported by Compliance Services International (CSI)

Y. Luo, D. Young, *Organizers*

J. Gan, K. S. Goh, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 ENVR **551.** Agricultural and urban pesticide signatures in wadeable streams from regional stream-quality studies. **L.H. Nowell**, B.J. Mahler, P.W. Moran, M. Shoda, J.E. Norman, P.C. Van Metre, W.W. Stone

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

1:55 ENVR **552.** Reconnaissance study of current-use pesticides in 12 urban and agricultural surface water sites in California. **M.L. Hladik**, J. Orlando

2:15 ENVR **553.** Pesticides in wastewater: Linking pesticide use patterns to sewershed monitoring results. **J. Teerlink**, R. Budd, Y. Xie, C. Alaimo, T.M. Young

2:35 ENVR **554.** Influence of rainfall event characteristics on urban pesticide runoff. **A. Gorgoglione**, F. Bombardelli, T.M. Young

2:55 ENVR **555.** Concentrations of synthetic pyrethroids in surface water and sediment from agricultural and urban land use areas. **J. Giddings**, J. Frew, D. Campana, J. Wirtz, B. Finch

3:15 Intermission.

3:35 ENVR **556.** Passive samplers for *in situ* monitoring of pesticides in urban surface water. **J. Gan**, W. Lao, C. Liao, A. Xue, J. Richards, K.A. Maruya

3:55 ENVR **557.** Continuous Low Level Aquatic Monitoring (C.L.A.M.) samplers for organic contaminant screening in urban runoff: Development of an analytical approach. **M. Vasquez**, S. Mohammed, H. Tsai, G. Cho, M. Ensminger

4:15 ENVR **558.** Analyses of polar pesticides and glyphosate in Mekong Delta. **N. Tran-Thi**, M. Do, L. Truong, T. Nguyen, T. Nguyen, Q. Chau, L. Tran, D. Orange, **P. Behra**

4:35 ENVR **559.** Environmental monitoring of systemic insecticides in surface water ecosystems: Development and application of an ultrasensitive and automated analytical method. **J.M. Montiel León**, S. Vo Duy, G. Munoz, M. Amyot, S. Sauvé

4:55 ENVR **560.** Desorption of known persistent organic pollutants from atmospheric dust and black carbon into aquatic ecosystems. **T. Togashi**, **C. Bowyer**, R.A. Lyons

5:15 Concluding Remarks.

Section B

San Francisco Marriott Marquis

Salons 12/13

Advances in Resource Recovery & Conservation in Water Systems

Cosponsored by AGFD, CEI and GEOC

S. Ahuja, L. M. Blaney, T. H. Boyer, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:40 ENVR **561.** Urea hydrolysis characterization and inhibition by chemical addition. **H. Ray**, D. Saetta, T.H. Boyer

2:00 ENVR **562.** Urea hydrolysis inhibition in waterless urinals for water conservation and nutrient recovery. **D. Saetta**, T.H. Boyer

2:20 ENVR **563.** Electrochemical stripping to recover nitrogen from source-separated urine. **W.A. Tarpeh**, K.L. Nelson

2:40 ENVR **564.** Life cycle comparison of urine source separation and centralized wastewater treatment. **T.H. Boyer**, K. Landry

3:00 Intermission.

3:20 ENVR **565.** Advanced spatial modeling and lifecycle assessment for real world implementation of decentralized nitrogen recovery. **O. Kavvada**, W.A. Tarpeh, A. Horvath, K.L. Nelson

3:40 ENVR **566.** Solution to pollution is not dilution: An integrated system for total nutrient recovery from source separated urine. **N. Jagtap**

4:00 ENVR **567.** Mechanisms and modeling of pathogen fate in pilot scale nutrient recovery reactors. **H. Bischel**, K. Udert, T. Kohn

4:20 ENVR **568.** Physical-chemical interactions of biochar and pharmaceuticals in synthetic urine. **A. Solanki**, T.H. Boyer

4:40 ENVR **569.** Fate of human BK polyomavirus through urine diverted for fertilizer. **H. Goetsch**, N. Love, M. Imperiale, K. Wigginton

5:00 Concluding Remarks.

Section C

San Francisco Marriott Marquis

Salons 14/15

Contaminants in Urban & Coastal Estuarine Ecosystems

Advanced Analytical Techniques to Assess Chemical Profiles

Cosponsored by AGRO

K. L. Armbrust, G. P. Cobb, P. Saranjampour, *Organizers*, *Presiding*

1:30 ENVR **570.** Combining chemical and bioanalytical methods to screen for emerging contaminants in California's receiving waters. **K.A. Maruya**, A. Mehinto, M. Raphael, E.D. Nelson, E. Hoh, S.A. Snyder, R. Fadness, J. Lyons

1:55 ENVR **571.** Regional trends in sediment quality in southern California: Responses to multiple stressors. **S. Bay**, N.G. Dodder, D. Gillett, K. Schiff

2:20 ENVR **572.** Examining urban metabolism and contaminants of emerging concern in coastal environments: A pilot study in Hong Kong and Taipei. **S. Burket**, J. Zheng, K. Chambliss, S. Chung, B.W. Brooks

2:45 ENVR **573.** Dissolved PAHs and PBDEs in the Narragansett Bay Watershed using passive polyethylene samplers. W. Zhao, M. Khairy, M. Cai, **R. Lohmann**

3:10 Intermission.

3:30 ENVR **574.** Ecotoxicological assessment of Polycyclic Aromatic Hydrocarbons (PAHs) and metals in the Mississippi River coastal watershed and offshore shoaling regions of the northern Gulf of Mexico. **L. Basirico**, R.J. Portier, H. Rockett

3:55 ENVR **575.** Quantifying Polycyclic Aromatic Hydrocarbons (PAHs) distribution and accumulation in coastal Louisiana using natural radioisotope tracers. **K. Maiti**, P. Adhikari, W. Bam

4:20 ENVR **576.** Assesment of emerging contaminants from wastewater treatment systems along Louisiana coastal and estuarine waterways. **M.S. Miles**

4:45 ENVR **577.** Stereoisomer-specific distribtuion of 1,2,5,6,9,10-hexabromocyclododecane and 1,2-dibromo-4-(1,2-dibromoethyl)cyclohexane in sediment and marine organisms from the South China Sea. **Y. Ruan**, X. Zhang, J.C. Lam, B. Zhu, P.K. Lam

5:10 ENVR **578.** Distribution and abundance of microplastic pollution on Sandy Hook Bay beaches is higher than on New Jersey coastal beaches. **K. Veasey**, S. Rosenstein

Section D

San Francisco Marriott Marquis

Golden Gate C1

Novel Membrane Materials & Processes for Water Purification

D. Jassby, B. Mi, *Organizers*, *Presiding*

1:30 ENVR **579.** Novel membranes with special wetting properties for anti-fouling and anti-wetting membrane distillation. Z. Wang, Y. Huang, **S. Lin**

2:00 ENVR **580.** Accurately determining convective heat transfer coefficients in membrane distillation cassettes. **M.S. Mauter**, M. Leitch, G. Lowry

2:20 ENVR **581.** Modification of permeate surface by hydrophilization to enhance flux in membrane distillation for desalination. **S. Ragunath**, S. Roy, S. Mitra

2:40 ENVR **582.** Desalting water with electric double-layers: Assessing impacts of material chemistry and operation strategies on capacitive deionization energy consumption and cost. S. Hand, **R. Cusick**

3:00 Intermission.

3:20 ENVR **583.** Sunlight enables reduced graphene oxide/bacterial nanocellulose ultrafiltration membranes to resist biofouling. **Y. Jun**, Q. Jiang, D. Ghim, S. Tadepalli, H. Kwon, K. Liu, Y. Min, J. Luan, S. Singamaneni

3:50 ENVR **584.** Surfactant-stabilized oil separation from water using ultrafiltration and nanofiltration. **X. Zhu**, A.V. Dudchenko, D. Jassby

4:10 ENVR **585.** Integration of reactive ceramic membrane with ozonation for advanced treatment of reclaimed water. **X. Zhang**

4:30 ENVR **586.** Novel nanohybrids enables microwave radiation to disinfection water. **N.B. Saleh**

4:50 ENVR **587.** Integration of *in-situ* ozonation and ceramic UF membrane for effective algae and MC-LR removal and membrane fouling control in the treatment of algal-rich water. **Z. Zhang**, Y. Tao, X. Zhang

Section E

San Francisco Marriott Marquis

Sierra A

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

X. He, D. Minakata, K. E. O'Shea, X. Quan, *Organizers*

D. D. Dionysiou, G. Li Puma, *Organizers*, *Presiding*

A. Ghauch, *Presiding*

1:30 ENVR **588.** Degradation of antibiotics in UV-persulfate activated systems: Application to Chloramphenicol. **A. Ghauch**, M. Amasha, A. Baalbaki, R. El Asmar, O. Tantawi

2:05 ENVR **589.** Electrochemical enhancement of oxidation process using persulfate activated by nanosized zero-valent iron. **C. Kim**, I. Hwang

2:30 ENVR **590.** Selective degradation of sulfamethoxazole by peroxymonosulfate without activating agents: Self-activation and nonradical pathways. R. Yin, **W. Guo**, H. Wang, J. Chang, N. Ren

2:55 ENVR **591.** Activation of persulfate with vanadium species for PCBs degradation: A mechanistic study. **G. Fang**, W. Wu, C. Liu, Y. Deng, D. Zhou

3:20 Intermission.

3:35 ENVR **592.** Effect of synthesis parameters in the removal of 4-chlorophenol under visible light irradiation using ammonium iron (II) sulfate-doped nano-titania photocatalyst. **F.A. Villaluz**, M. Lu, M.G. de Luna

4:00 ENVR **593.** :β-Bi_2O_3 thin films on different substrates for photodegradation of organic dyes. **T. Gadhi**, L. Gómez, M. Bizarro, **J.C. Medina**, P. Jagdale, A. Hernández-Gordillo, A. Tagliaferro, S.E. Rodil

4:25 ENVR **594.** Evaluation of heterogeneous photocatalysis degradation of ketoprofen in aqueous solution with catalysts TiO_2/Mo/Ag. **A. Suarez**, V. Rodriguez Gonzalez, E.F. Sarria, L. Clavijo

4:50 ENVR **595.** Micromotors as tools for efficient water decontamination. **D. Vilela Garcia**, J. Parmar, S. Sanchez

5:15 Concluding Remarks.

Section F

San Francisco Marriott Marquis

Sierra B

Aquatic Photochemistry

Cosponsored by GEOC

Financially supported by AEESP

W. Arnold, K. P. McNeill, *Organizers*

V. Lin, *Organizer, Presiding*

1:30 ENVR **596.** Characterizing the role of photochemical processes in the oxidation of hydrocarbons released during the Deepwater Horizon disaster. **C.P. Ward**, C. Reddy

1:50 ENVR **597.** Time dependence of aldehyde and ketone photoproduct generation from crude oil-seawater systems under solar irradiation. **X. Cao**, M.A. Tarr

2:10 ENVR **598.** Steric hindrance reduces aquatic photochemical transformation rates of alkylated sulfur heterocycles. **P. Saranjampour**, K.L. Armbrust, B. Marx

2:30 ENVR **599.** Photolysis of aromatic pollutants in salty water and ice. **T.F. Kahan**, A. Stathis, P. Malley, J. Grossman

2:50 ENVR **600.** Petroleum provides model compounds to assess the compositional and structural controls of dissolved organic matter photoreactivity. **P. Zito**, M.A. Tarr, D.C. Podgorski

3:10 Intermission.

3:20 ENVR **601.** Investigating the photochemical pathways of organic sulfur in forming COS and CS_2 in natural waters. **M. Modiri Gharehveran**, A. Shah

3:40 ENVR **602.** Counter-ions influence nitrate photolysis yields through altering interfacial concentrations. **K.M. Callahan**, D. Tobias

4:00 ENVR **603.** Characterization of photooxidants in atmospheric particles. **R. Kaur**, C. Anastasio

4:20 ENVR **604.** Is gas-aerosol particle interface the same as the air/water interface? **Y. Rao**, Y. Wu, X. Li, Y. Wu, Y. Qian, H. Dai

4:40 ENVR **605.** From the desert to the city: Dust as a photochemical source of hydroxyl radical and singlet oxygen in aqueous aerosol. **S.A. Styler**, S.R. Schneider, C.D. Cote

Section G

San Francisco Marriott Marquis

Sierra C

Innovative Materials & Technologies for Sustainable Water Purification

Photocatalytic

Cosponsored by CEI

E. L. Cates, B. P. Chaplin, J. Choe, J. Liu, W. Zhang, *Organizers*

D. Shuai, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ENVR **606.** Boosting the photocatalytic activity of m-$BiVO_4$ with Pd nanodomains and BiOBr nanosheets dual heterojunction: Highly effecient photocatalytic degradation of polychlorinated biphenyls. **E. Zahran**, M. Palmai, S. Angaramo, M.R. Knecht, L. Bachas

1:55 ENVR **607.** Tailored graphitic carbon nitride: Selective production of oxidative species and applications for organic micropollutant removal. **Q. Zheng**, D. Shuai

2:15 ENVR **608.** Synthesis and application of highly reductive TiO_2-based photocatalysts for hexavalent chromium and nitrate removal. **G. Chen**, H. Liu

2:35 ENVR **609.** Microreactor-inspired photocatalytic PBR for intensified solar photocatalysis: A study of the effects of packing material on light absorption. **B. Ramos**, S. Ookawara, A.S. Teixeira

2:55 Intermission.

3:10 ENVR **610.** Towards multifunctionality in water treatment: Developing photoactive selective adsorbents for inorganic contaminants using nano-enabled biomaterials. **L. Pincus**, J. Yamani, J.B. Zimmerman

3:30 ENVR **611.** Designing photocatalytic nano-adsorbents with greater specificity through shape and size using advanced spectroscopy techniques. **A.W. Lounsbury**, N. Billmyer, J. Yamani, D. Peak, J.B. Zimmerman

3:50 ENVR **612.** Physical and chemical characterization of iron (III) oxide produced by SORAS technique for the removal of arsenic in drinking water. **E. Araya**, J. Valverde-Cerdas, J.M. Cubero-Sesin, D. Méndez, **L.G. Romero**

4:10 ENVR **613.** Antimicrobial applications of visible-light-responsive photocatalysts. **H. Shen**, D. Shuai

Section H

San Francisco Marriott Marquis

Sierra J

Poly- & Per-Fluoroalkyl Substances: Where, What, When, Why, Who & How

K. Chu, L. S. Lee, J. Liu, V. Yingling, *Organizers*, *Presiding*

1:30 ENVR **614.** Encapsulation of legacy and emerging perfluoroalkyl substances by cyclodextrins. M.J. Weiss-Errico, Z. Hopkins, D. Knappe, **K.E. O'Shea**

1:55 ENVR **615.** Protective effects of β-cyclodextrin in biological systems contaminated with perfluoroalkyl substances. **M.J. Weiss-Errico**, K.E. O'Shea

2:20 ENVR **616.** Novel approach to the enhancement of PFAS adsorption in groundwater systems. **Y. Aly**, M.F. Simcik

2:45 ENVR **617.** Selective and fast adsorption of perfluorooctane sulfonate from wastewater by magnetic fluorinated vermiculite. **S. Deng**, P. Meng, G. Yu

3:10 Intermission.

3:40 ENVR **618.** Abiotic transformation of perfluorooctane sulfononate by catalyzed permanganate under amenable in-situ conditions. **S. Park**, L.S. Lee

4:05 ENVR **619.** Remediation of per- and polyfluoroalkyl substances using heat-activated persulfate. **T. Bruton**, D.L. Sedlak

4:30 ENVR **620.** Remediation of perfluorinated surfactants in groundwater by injection of nanoscale zerovalent iron particles. **Y. Zhang**, Y. Zhi, J. Liu, S. Ghoshal

4:55 ENVR **621.** Degradation of Poly- and Per-Fluoroalkyl Substances ($PFAS_s$) using photocatalyst zinc oxide. K. Chu, **Y. Shao**

5:20 Concluding Remarks.

Section I

San Francisco Marriott Marquis

Sierra K

Whole Organism Metrology to Support Nanotoxicology Research in the Environment

S. K. Hanna, M. Johnson, *Organizers*

B. C. Nelson, C. M. Sims, *Organizers*, *Presiding*

1:30 ENVR **622.** Development of correlative optical microscopy and focused ion beam tomography for quantitation of metal nanoparticles in whole cells. **K. Jeerage**, A. Sanders

1:55 ENVR **623.** Single cell ICP-MS: Quantifying exposure and dose of gold and silver nanoparticles to freshwater algae. **R. Merrifield**, J. Lead, C. Stephan

2:20 ENVR **624.** Optofluidic Surface Enhanced Raman Spectroscopy (SERS) interrogation for targeted detection of individual cells. **M. Willner**, D. Graham, M. Zagnoni, P.J. Vikesland

2:45 ENVR **625.** Quantitative analysis of the physicochemical properties of cerium oxide nanomaterials and their influence on nano-bio interactions. **C.M. Sims**, R.A. Maier, A.C. Johnston-Peck, J.M. Gorham, S.K. Hanna, V.A. Hackley, B.C. Nelson

3:10 Intermission.

3:25 ENVR **626.** Transfer and accumulation of TiO_2 nanoparticles along a marine benthic food chain. J. Zhao, Z. Wang, **B. Xing**

3:50 ENVR **627.** Toxicity studies of silver nanoparticles on the anaerobic sulfate reducing bacteria *Desulfovibrio alaskensis*. **M.O. Montes**, J.M. Snitker

4:15 ENVR **628.** Effects of pH and dissolved organic carbon on the toxicity of silver nanowires to *Daphnia magna*: Acute toxicity and spICP-MS measurement of silver nanowire uptake. **L.D. Scanlan**, M.D. Montano, N. Karunaratne, M. Eng, T. Cun, J.Y. Hsu, C. ter Haar, B. Gilbert, C. Vulpe

4:40 ENVR **629.** Monitoring toxicity of oral magnetite nanoparticles *in vivo* using drosophila melanogaster. **X. Bi**

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

Sponsored by GEOC, Cosponsored by COLL, ENVR and NUCL

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Fundamental Structure-Activity Relationships: The Interface of Operando with Physical Sciences

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Elucidation of Mechanisms & Kinetics on Surfaces

Mechanisms: Hydrogenation

Sponsored by CATL, Cosponsored by COLL and ENVR

WEDNESDAY EVENING

Section A

Moscone Center

Hall D

Accurate Mass/High Resolution Mass Spectrometry for Environmental Monitoring & Remediation

Cosponsored by ANYL

T. Anumol, R. Marfil-Vega, T. M. Young, *Organizers*

6:00 - 8:00

ENVR **630.** Screening and quantitation of micro-pollutants from sewage water in the process of bank filtration using UHPLC-HRAM. **E. George**

ENVR **631.** Assessment of biotransformation of macrolide antibiotics using target and non-target analyses by ultraperformance liquid chromatography/quadrupole-time-of-flight mass spectrometry and antibiotic bioassay. **S. Terzic**, N. Udikovic-Kolic, I. Krizman, I. Senta, I. Mihaljevič, T. Smital, M. Ahel

ENVR **632.** Withdrawn

ENVR **633.** Polypropylene glycol surfactants and their degradation products as potential indicator compounds for shallow groundwater impacted by hydraulic fracturing fluids. **J.D. Rogers**, I. Ferrer, E.M. Thurman, J. Rosenblum, A.R. Bielefeldt, J.N. Ryan

ENVR **634.** Microcystin screening in water samples using LC-MS/MS and triggered information dependent acquisition for non-targeted variant detection. **R.A. Trenholm**, B. Vanderford

ENVR **635.** Levels, profiles and potential risks of dioxins and dioxin-like compounds in atmosphere surrounding industrial sources. **G. Liu**, **M. Zheng**, L. Yang, R. Jin, Q. Zhu

ENVR **636.** Determination and quantitative of plant metabolites by using triple quadrupole liquid chromatography coupled to mass spectrometry. **Y. Huang**, L. Zhao, A.S. Adeleye, T. Anumol, A.A. Keller

ENVR **637.** Withdrawn

ENVR **638.** Use of gas chromatography orbitrap mass spectrometry for small molecule discovery: Iodinated disinfection byproducts as case study. C. Postigo, C. Cojocariu, S.D. Richardson, **P. Silcock**, D. Barceló

ENVR **639.** Python script to streamline non–targeted GC×GC/TOFMS data analysis of remediated soil samples. **I. Titaley**, O. Ogba, L. Chibwe, E. Hoh, P. Cheong, S.L. Simonich

Section A

Moscone Center

Hall D

Advances & Applications in Water Sensing Technologies for Drinking Water, Re-Use, Agri-Tech & Research

P. L. Schorr, *Organizer*

6:00 - 8:00

ENVR **640.** Withdrawn

ENVR **641.** Nano-sized TiO_2 thin film synthesis and characterization on quartz slides, borosilicate beads and quartz cylinders for use in photocatalytic degradation of organic contaminants. **M. Russell**, S.R. Kanel, D. Kempisty

ENVR **642.** Engineering analysis of water reuse through water sensing spectrophotometers. **P.L. Schorr**

Section A

Moscone Center

Hall D

Advances in Resource Recovery & Conservation in Water Systems

S. Ahuja, L. M. Blaney, T. H. Boyer, *Organizers*

6:00 - 8:00

ENVR **643.** Effect of humic analogue on microbial leaching of iron from hematite into seawater. **A. Aneksampant**

ENVR **644.** Phosphorus recovery using pelletized adsorptive materials: Study of desorption for potential reuse. **E. Martin**, M. Nadagouda, S. Chae

ENVR **645.** Integrated seawater aquaculture and agriculture as an avenue for food and energy security in arid regions. **Z. Almheiri**

ENVR **646.** Efficacy of Hydrotalcite-based nanocomposites for sorbing heavy metal in industrial wastewater. **Y. Li**, J. Ma, P.J. Alvarez

ENVR **647.** Phosphate ion exchange on cross-linked cationic surfactant micelles across dialysis membranes. **M. Chen**, C.T. Jafvert

‡ *Cooperative Cosponsorship*

Section A

Moscone Center
Hall D

Applications of Cheminformatics & Computational Chemistry in Environmental Health

C. Grulke, A. J. Williams, *Organizers*

6:00 - 8:00

ENVR **648.** Integrating chemometrics and computational chemistry in the workflow of suspect screening analysis of polycyclic aromatic hydrocarbon biotransformation products. **I. Titaley**, L. Chibwe, K.R. Glaesemann, P. Cheong, S.L. Simonich

ENVR **649.** Molecular dynamics study of the influence of activated carbon pore structures on dioxin adsorption. **F. Gao**, S. Qu, C. Liu, H. Li, B.J. Teppen, C.T. Johnston, S. Boyd

ENVR **650.** Progress towards a general model to predict hydroxylated polycyclic aromatic hydrocarbon stabilities. **D. Walden**, I. Titaley, O. Ogba, S. Simonich, P. Ha-Yeon Cheong

ENVR **651.** Delivering an informational hub for data at the National Center for Computational Toxicology. **A.J. Williams**, C. Grulke, J. Smith, K. Mansouri, A. McEachran, G. Patlewicz, J. Fitzpatrick, A. Richard, J. Edwards

Section A

Moscone Center
Hall D

Aquatic Photochemistry

Cosponsored by GEOC

Financially supported by AEESP

W. Arnold, V. Lin, K. P. McNeill, *Organizers*

6:00 - 8:00

ENVR **652.** FT-ICRMS analysis of photochemically degraded and burned surrogate oil. **M.D. Seivert**, C.A. Davis, A.M. McKenna, Y. Corilo, R.A. Snyder, W.H. Jeffrey, P.P. Vaughan

ENVR **653.** Direct and indirect photochemical transformation of imidazolium, pyridinium, pyrrolidinium, and piperidinium ionic liquids. **S.G. Pati**, W. Arnold

ENVR **654.** Formation of brown carbon in snow and ice through SOA-like chemistry. **M. Barr**, A.M. Grannas, V. Boschi

ENVR **655.** Photochemical transformation of nicotine in the wastewater effluent. **L. Lushi**, S. Yan, W. Song

ENVR **656.** Photoreactivity of plant elicitor acibenzolar S-methyl in solutions and on plant surfaces. **M. Sleiman**, M. Stawinoga, S. Wang, P. Goupil, C. Richard, P. De Sainte Claire

ENVR **657.** Removal of arsenic by UV photoreduction in the presence of dithionite. **B. Jung**, A. Abdel-Wahab

ENVR **658.** Photochemical reactions of hematite-soot mixtures in various environmentally representative scenarios. **J. Rodriguez**, J. Rodriguez, A. Reddy, H. Casique, A.M. Johansen

ENVR **659.** Fluorescence spectroscopy for determining photochemical degradation rates of natural and industrial crude oil with DOC and GC×GC/TOF-MS analysis. **K. Snyder**, N. Mladenov, A. Nour, C. Campbell, M. McConnell, R. Luna, E. Hoh

ENVR **660.** Modeling singlet oxygen production by dissolved organic matter. **J.R. Laszakovits**, Y. Chin, A. MacKay, **C.M. Sharpless**

ENVR **661.** Exploration of the role of ambient conditions in organic aerosol growth via photosensitized oxidation of VOCs. **M. Galloway**, M.G. Ippolito, J.M. Ackendorf, A. Sager

ENVR **662.** Antioxidant response to singlet oxygen production under light stress on the polyphasic rise of chlorophyll a fluorescence induction curves of *Botryococcus braunii*. **F.M. Joaquin**, G. Guihurt, K. Doble, V. Barcelo Bovea, K. Griebenow

ENVR **663.** Biological toxicity of extracts from photochemically degraded crude oil water accommodated fractions. **P. Bann**, **S. Bifulco**

ENVR **664.** Fractionation and biological toxicity studies of crude oil water accommodated fractions with dispersant. **C. Brannon**, P. Bann, S. Bifulco, J. Fair, M.D. Seivert, W.H. Jeffrey, P.P. Vaughan

Section A

Moscone Center
Hall D

Bioprocesses for Engineered Nanomaterials in Soil-Plant Systems

J. C. White, B. Xing, Y. Yang, *Organizers*

6:00 - 8:00

ENVR **665.** *In-situ* study of the evolution of quantum dots in contact with the biofilm/mineral interface. **M. Desmau**, **G. Alexandre**, C. Levard, G. Ona-Nguema, V. Vidal, J. Stubbs, G. Charron, Y. Sivry, M.F. Benedetti

ENVR **666.** Effects of carbonaceous nanomaterials on soil-grown soybean and its symbiosis with nitrogen-fixing bacteria: A mesocosm study. **Y. Wang**, D.C. Bouchard, R.M. Nisbet, J.P. Schimel, J.L. Gardea-Torresdey, P. Holden

ENVR **667.** Molecular mechanisms underlying biotransformation of carbon nanotubes by *Mycobacterium vanbaalenii* PYR-1. **Y. You**, J. Angermann, B. Xing, S. Kim, O. Kweon, C. Cerniglia, Y. Yang

Section A

Moscone Center
Hall D

Chemical Principles of Environmental, Cellular & Organismal Nanotoxicology

Cosponsored by COLL

C. Celle, L. L. Charlet, B. Gilbert, S. Lehman, J. Simonato, C. Vulpe, *Organizers*

6:00 - 8:00

ENVR **668.** Stability and cytotoxicity of synthesized CeO_2 nanoparticles in water. **Y. Lin**, L. Shen, Y. Shih

ENVR **669.** Predictive insight into the silver nanomaterial protein corona fingerprint. **M.R. Findlay**, **D.N. Freitas**, M. Mobed-Miremadi, **K. Wheeler**

ENVR **670.** Exploring impacts of complex nanomaterials using the nematode *C. elegans*. **N. Niemuth**, M. Hang, X. Zhang, R.J. Hamers, C.J. Murphy, R. Klaper

ENVR **671.** Characterization of biophysical characteristics that impact individual peptide binding to an engineered nanomaterial within a complex blood protein corona. **M. Nguyen**, **K. Wheeler**

ENVR **672.** Modeling the environmental fate of graphene oxide and its transformation products in surface waters. **D.C. Bouchard**, B. Avant, X. Chang, L. Guiney, Y. Han, M. Henderson, M. Hersam, C. Knightes, S. Martin, J. Spear, R.G. Zepp

ENVR **673.** Characterization of the dissolution properties of copper oxide nanoparticles in cell culture media and their effects on *in-vitro* toxicity. **S. Jang**, W. Kim, E. Cho, S.I. Yang

ENVR **674.** Inhibition effects of silver nanoparticles and ions on toxic airborne fungi. **E. Cho**, J. Lee, S.I. Yang

ENVR **675.** Nanotoxicology of NMC, PAH-AuNP, Citrate-AuNP and *D. melanogaster*. **B. Curtis**, M. Hang, R.J. Hamers, X. Zhang, C.J. Murphy, R. Klaper

Section A

Moscone Center
Hall D

Chemistry & Application of Advanced Oxidation Processes for Water Detoxification, Treatment & Reuse

Financially supported by AEESP

D. D. Dionysiou, X. He, G. Li Puma, D. Minakata, K. E. O'Shea, X. Quan, *Organizers*

6:00 - 8:00

ENVR **676.** Photodegradation of antibotic in organic matter solution using H_2O_2/UV process. **A.S. Batista**, N. Silva, L. Gil da Barbara, I.V. Corrêa, A.S. Teixeira

ENVR **677.** Degradation of a toxic molecule in industrial effluents using UV/PS activated systems: Application to o-toluidine. **A. Ghauch**, A. Baalbaki, M. Amasha, S. Al Hakim, Y. Nehme, R. El Asmar

ENVR **678.** Withdrawn

ENVR **679.** Withdrawn

ENVR **680.** Withdrawn

ENVR **681.** Effects of bulk water temperature on PAH degradation by ultrasonically activated persulfate. **W.P. Fagan**, J. Zhao, L.K. Weavers

ENVR **682.** Withdrawn.

ENVR **683.** Gaseous VOC abatement in a Circulating Fluidized Bed (CFB) riser reactor: A Computational Fluid Dynamics (CFD) modeling approach. **D. Matsumoto**, L. Diniz, J.L. de Paiva, A.S. Teixeira, R. Guardani, T. Hewer

ENVR **684.** Photocatalytic decomposition of imidacloprid by TiO_2-Fe_3O_4 nanocomposite in a PV-UV-LED continuous photoreactor. **M. Eskandarian**, M. Fazli, M. Rasoulifard

ENVR **685.** Natural enhancement of Solar Disinfection (SODIS) via the photo-Fenton process towards bacterial and chemical contaminant elimination in developing countries. **S. Giannakis**, C. Pulgarin

ENVR **686.** Photocatalytic degradation of C.I. basic red 46 in thin film fixed bed photoreactor: Non linear regression analysis and intermediates. **M. Berkani**, M. Bouhelassa, B. Abdelkrim, M. Bouchareb, Y. Kadmi

ENVR **687.** Influence mechanisms of textile-dyeing sludge characteristics on degradation of anilines by integrated ultrasound-permanganate treatment. **X. Ning**, **J. Liang**, T. An, J. Sun, X. Lu, Y. Zhang

ENVR **688.** Efficient degradation of DBP by magnetic nano-fiber GO-$MnFe_2O_4$ as ozonation catalyst in the water. **Y. Ren**, J. Ma, H. Zhang

ENVR **689.** Chloroperoxidase oxidative transformation of roxarsone. **Y. Tan**, X. Wang, K.E. O'Shea

ENVR **690.** Bioactivity-oriented approach to investigate fate and transformation of selected personal care products during chlorination. L. Li, **W. Han**, K. Yeung

ENVR **691.** Simultaneous photocatalytic Cr(VI) reduction and ciprofloxacin oxidation over TiO2/Fe0 composite under aerobic conditions: Performance, durability, pathway and mechanism. **Z. Diao**

ENVR **692.** Elimination of analgesic residuals in water by ultrasound and ultrasound-assisted catalytic processes. **A. Ziylan Yavas**, N.H. Ince

ENVR **693.** Photocatalytic removal of toluene in a TiO_2 /SiO_2 circulating fluidized bed reactor. **L. Diniz**, D. Matsumoto, T. Hewer, A.S. Teixeira, J.L. de Paiva, R. Guardani

ENVR **694.** Withdrawn.

ENVR **695.** Application of iron mining residue for heterogeneous photo-fenton degradation of sulfathiazole and sulfamethazine. **S.C. Ayala**, P. Hammer, R. Pupo Nogueira

ENVR **696.** 17-Ethinylestradiol degradation promoted by persulfate activated with UV-light. **C. Rackov**, A.G. Camara, T.A. Ferreira, H.N. Maia de Oliveira, M. Vianna, O. Chiavone-Filho, C.A. Oller do Nascimento

ENVR **697.** Semiconductor nanomaterials for solar photocatalytic activity. L. Gustin, B. Dallakoti, X. Cao, **M.A. Tarr**

ENVR **698.** Toxicity removal by electro-peroxone process. **D. Amado Piña**, G. Roa Morales, G. Santana Martínez, C. Barrera-Díaz, P. Balderas-Hernández, R. Romero Romero, **R. Natividad**

ENVR **699.** Ag nanoparticles stabilized with starch deposited on the TiO_2 and TiO_2-CeO_2 systems. **J.C. Arevalo Perez**, J.G. Torres Torres, I. Sanchez Lombardo, A. Cervantes, A. Cordero, A.A. Silahua

ENVR **700.** Probing electron trapping energy states of TiO_2-WO_3 composites and their consequences on photocatalytic activity for bisphenol A removal. G. Zerjav, S. Arshad, P. Djinovic, **A. Pintar**

ENVR **701.** Removal of alkyl nitrate chemical contaminants in wastewaters using advanced oxidative processes. **S. Arciva**, B. Daws, S.P. Mezyk, M.P. Schramm

ENVR **702.** Bromine atom reactions under advanced oxidation process conditions. **A. Lechner**, **S.P. Mezyk**

ENVR **703.** Withdrawn.

ENVR **704.** Design of hierarchical photocatalyst for waste water treatment. **B. Barbero**, C.M. Parlett, A.F. Lee, K. Wilson

ENVR **705.** Withdrawn.

ENVR **706.** QSAR prediction of rate constants for the reaction of ozone with organic compounds using quantum chemical descriptors beyond HOMO. **P.R. Tentscher**, U. von Gunten

Section A

Moscone Center
Hall D

Chemistry of Water Treatment from Sorption to Taste & Odor: Symposium honoring the Contributions of Mel Suffet

M. J. McGuire, J. A. Pedersen, F. L. Rosario, *Organizers*

6:00 - 8:00

ENVR **707.** Photochemical reactivity of thermally-altered water soluble organic matter. **K.D. Couch**, F.L. Rosario, G. McKay, Y. Yu, A. Retuta

ENVR **708.** Characterizing the properties and release kinetics of dissolved organic carbon from thermally treated soils in arid climates. **A. Retuta**, Y. Yu, F.L. Rosario

ENVR **709.** Do all reduced sulfur compounds in foul air vary in the same manner over a daily fluctuation in the wastewater treatment process? **T. Vitko**

Section A

Moscone Center
Hall D

Clay Minerals Selectivity & Its Environmental Applications

M. ElSayed, *Organizer*

6:00 - 8:00

ENVR **710.** Use of NMR carbon-type distributions to assess the extent of preferential adsorption of natural organic matter components. M. Khalaf, G. Chilom, **J.A. Rice**

ENVR **711.** Sorption of substituted pyridines to aluminosilicate clays: Building predictive models for cationic amines. **D. Haas Freeman**, J. Sullivan, D. Vasudevan

Section A

Moscone Center
Hall D

Contaminants in Urban & Coastal Estuarine Ecosystems

Cosponsored by AGRO

K. L. Armbrust, P. Saranjampour, *Organizers*

6:00 - 8:00

ENVR **712.** Determination of total copper concentration and copper speciation in Humboldt Bay, California through use of competitive ligand exchange-adsorptive cathodic stripping voltammetry. **M.A. Amezcua**, N. Tuttle, M.P. Hurst

ENVR **713.** Soil degradation and sorption of azithromycin in simulated California river and river bed conditions. **M.L. Maier**, R.S. Tjeerdema

ENVR **714.** Anti-depressant and legacy contaminant fate in the Gulf of Mexico. **J. Landry**, K.L. Armbrust

ENVR **715.** Potential mechanisms of 2,6-dichloro-4-nitroaniline (Dicloran) phototoxicity to *Pimephales promelas* (Fathead Minnow). **E.N. Vebrosky**, K.L. Armbrust

ENVR **716.** Analysis of metabolites of Polycyclic Aromatic Hydrocarbons (PAH) in fish bile: A 15-year temporal survey of PAH exposure in Puget Sound, WA. **C. Gallagher**, D. Da Silva

ENVR **717.** From sediment to top predators: Broad exposure of polyhalogenated carbazoles in San Francisco Bay (U.S.A.). Y. Wu, H. Tan, R.A. Sutton, **D. Chen**

ENVR **718.** Withdrawn.

Section A

Moscone Center
Hall D

Contaminants of Emerging Concern in Natural & Engineered Systems

Cosponsored by AGRO, ANYL and CEI

L. M. Blaney, A. J. Hernandez, *Organizers*

6:00 - 8:00

ENVR **719.** UV-driven antibiotic-to-antibiotic transformation pathways and kinetics of sulfonamides. **D. Ocasio**, **H.A. Adejumo**, K. Mangalgiri, K. He, L.M. Blaney

ENVR **720.** Photolytic fate of organo-selenium and -tin chemicals and their carbon analogs in the natural environment. **M. Hopanna**, S. Steinly, L.M. Blaney

ENVR **721.** Photocatalytic degradation of 1,4-dioxane and trihalomethanes by zinc oxide. **M. Hwangbo**, Y. Shi, E. Claycomb, B.S. Abada, K. Chu

ENVR **722.** Occurrence and fate of low molecular weight aldehydes in potable water reuse systems. **E. Marron**, C. Prasse, D. Sedlak

ENVR **723.** Occurrence of phthalic acid esters and alkylphenols in the Asan Lake region, Korea. Y. Lee, T. Kim, J. Lee, W. Choe, **K. Zoh**

ENVR **724.** Withdrawn.

ENVR **725.** Enabling time dependent predictions of emerging organic chemicals in the environment using the OrganoFate model. **R. Thakar**, D. Elsbury, K. Garner, A.A. Keller

ENVR **726.** Toxicity and degradation of a polyalkylene glycol-based hydraulic fluid. **Y. Yang**, K.K. Das, R. Murnane, J. Hou, V. Edirveerasingam

ENVR **727.** Identification of PAH oxidation products on secondary organic aerosols. **A. Kramer**, S. Simonich, A. Zellenyuk, K. Suski, D. Bell

ENVR **728.** Hexachlorobutadiene in agricultural soils from the Yangtze River Delta of China. **J. Sun**, **X. Li**

ENVR **729.** Adsorptive removal of contaminants of emerging concern from water with imprinted zeolite carbon composites functionalized with extra-framework Cu^{2+}. **B. Fernandez-Reyes**, K.M. Gonzalez-Ramos, K. Ortiz-Martinez, A.J. Hernandez

ENVR **730.** Predicting sorption of anionic pharmaceuticals to soils: An evaluation of potential probe compounds. **L. Alper**, A. Lopez, D. Vasudevan

ENVR **731.** Characterizing in-situ methane-enhanced biostimulation potential for 1,4-dioxane biodegradation in groundwater. **V. Sadeghi**, D. Chiang, R. Mora

ENVR **732.** Withdrawn.

ENVR **733.** New analytical method for analysis of a broad range of chemicals found in Australian waters and wastewaters. **A. Kahl**

Section A

Moscone Center
Hall D

Environmental Chemistry: Undergraduate & Graduate Classroom, Laboratory & Local Community Learning Experiences

Cosponsored by ANYL and CHED

Financially supported by AEESP

M. A. Benvenuto, E. Roberts-Kirchhoff, *Organizers*

6:00 - 8:00

ENVR **734.** Seasonal differences in mercury concentrations in fish from Flint Creek, Alabama: Implications for monitoring. **P. Okweye**

ENVR **735.** Measurement of hazardous air pollutants with regard to environmental justice policy in the Atlanta metropolitan region. W. Hudson, D. Patel, **K. Zimmermann**

ENVR **736.** Adsorption of herbicide on the model solid/liquid interface. **P. Orlović-Leko**, K. Vidović, I. Ciglenečki

ENVR **737.** Localized surface plasmon resonance and electrochemical analysis of electron transfer mediators. **D. Panfilov**, P.W. Hall

ENVR **738.** Effects of wastewater treatment on Azithromycin. **E. Avila**, A. Hermelinda, M. Perri

ENVR **739.** Withdrawn.

ENVR **740.** Gas-phase mercury cycles during May at urban/industrial sites on Svalbard. **S. Le Cras**, M.H. Hermanson, A. Nikulina

ENVR **741.** Synthesis of a series of podand ligands all incorporating long-chain aliphatic moieties. **G. Nguyen**, J. Pothoof, S. Tinawi, M.A. Benvenuto

ENVR **742.** Analysis of mineral cosmetics with a handheld X-ray fluorescence analyzer. **S. Thomas**, **G. Nguyen**, D. Stokes, T. Tieu Ngo, M.A. Benvenuto, E. Roberts-Kirchhoff

Section A

Moscone Center
Hall D

From the Bench to the Field: Evaluating Innovative Remediation & Detection Technologies

S. R. Al-Abed, H. Henry, *Organizers*

6:00 - 8:00

ENVR **743.** Enhanced field screening methods of soil gas in petroleum hydrocarbon contaminated sites. **C.S. Chen**, C. Tien, C. Kuo

ENVR **744.** Evaluation of oxidizer hazard in sorbents used to solidify transuranic waste for the waste isolation pilot plant. **B.A. Crawford**, T. Hayes, J. Lucchini, C. Chancellor, C. Poulos

ENVR **745.** Development and demonstration of high pressure direct push jet injection for controlled emplacement of treatment agents in low-permeability geologic matrices. **N.D. Durant**, C. Ross, W. Slack

ENVR **746.** Utilization of multivariate analysis for evaluating geomaterial performance on fluoride removal from water. **E. Kim**, J. Park, S. Han, Y. Lim, K. Kong, J. Do

ENVR **747.** Identification and quantification of polycyclic aromatic hydrocarbon breakdown products in thermally remediated soil from the Wyckoff/Eagle Harbor Superfund site. **L. Santiago Delgado**, E.L. Davis, S. Simonich

ENVR **748.** Electrokinetic enhanced amendment transport at a contaminated field site. **D.M. O'Carroll**, A. Chowdhury, J. Gerhard, N. Head, A. Inglis, A. Nunez Garcia

Section A

Moscone Center
Hall D

General Posters

S. R. Al-Abed, S. O. Obare, *Organizers*

6:00 - 8:00

ENVR **749.** Removal of microcystin-LR using powdered activated carbon: Effects of water quality and activated carbon properties. **A. Bajracharya**, J.J. Lenhart

ENVR **750.** Adsorption of fluoride in aqueous solution using Jamun (Syzygium cumini) seed derived activated carbon. **R. Araga**, C. Sharma

ENVR **751.** Fabrication and characterization of surface-patterned thin-film composite membranes. **O. Heinz**, S.H. Maruf, M. Aghajani, A.R. Greenberg, Y. Ding

ENVR **752.** Image analysis for assessment of nanomaterial uptake and elimination kinetics. **T. Kefela**, M. Mortimer, P. Holden

ENVR **753.** Modification of graphene oxide with magnesium oxide: Synthesis, characterization, and demonstration with high-rate adsorption of methylene blue. **M. Heidarizad**, S.S. Sengor

ENVR **754.** Caffeine analysis of wastewater using online SPE-LC high resolution mass spectrometry. **S. Spence**, P.R. Gardinali

ENVR **755.** Correlation of chemical composition of wood smoke and diesel exhaust particulate matter with light absorbance and toxicity. **K. Kukowski**, B.C. Brinchmann, R. Cochran, J.A. Øvrevik, A. Kubatova

ENVR **756.** Factors affecting the fate of dissolved organic carbon in groundwater. **L.K. McDonough**, A. Baker, D. O'Carroll, M. Andersen

ENVR **757.** Comprehensive real-time fenceline monitoring using SIFT-MS. V.S. Langford, **B.J. Prince**, D.B. Milligan, T. Wilks, T. Potter

ENVR **758.** Removal of chromium(VI) and chromium(III) ions from aqueous solution using bio-char generated from agricultural waste products. **D.F. Gonzalez**, K. Flores, M. Gonzalez, A. Cantu, C. Serna, T.M. Eubanks, J.G. Parsons

ENVR **759.** Effect of absorber and desorber unit interactions on N-nitrosamine formation during amine-based carbon capture. **Z. Wang**, Z. Zhang, W. Mitch

ENVR **760.** Characterization of heavy metal adsorption using precipitates in acid mine water from abandoned metal mine. **J. Kim**, J. Kim, C. Seo, J. Seo, Y. Kim

ENVR **761.** Quantitative analysis of tetrabromobisphenol-A and tribromobisphenol-A in dust from consumer electronics. E. Gaulke, C.R. Butler, A. Schoffstall, L.E. Lowe, **J.E. Owens**

ENVR **762.** Comparison of the persistence of caffeine in constructed wetlands versus convention wastewater treatment systems. **P.R. Alvaro**, C. Tripp, M.P. Hurst

‡ *Cooperative Cosponsorship*

ENVR **763.** Reduction of ferric iron in aqueous soot slurries. H. Casique, A. Reddy, C. Neuman, **A.M. Johansen**

ENVR **764.** Detailed examination of particulate matter from waste vegetable oil biodiesel combustion: Oxidative potential relationships to fuel feedstock and blend ratio composition. **B. Holmen**, B. Rukavina, J. Kasumba, J. Reed, Y. Han, N.K. Fukagawa

ENVR **765.** Novel approaches to the study of bio-based products and anaerobic digestion per compost environment standard. E.J. Parish, G. Ren, H. Honda, **S. Lee**, Y. Lo

ENVR **766.** Novel development to the application of life cycle approach to design greener products. G. Ren, E.J. Parish, **H. Honda**, Y. Lo

ENVR **767.** Novel approaches to the application of estimation methods to reduce carbon emission on climate change. G. Ren, E.J. Parish, H. Honda, **Y. Lo**

ENVR **768.** Influence of dissolved organic carbon on mercury transport in watersheds affected by historical gold and mercury mining in northern California. **C.N. Alpers**, J.A. Fleck, M. Marvin-DiPasquale, G. Aiken

ENVR **769.** Identification of fungal genus level using DNA barcode method. **D. Kim**, D. Kang, J. Lee, E. Cho, S.I. Yang

ENVR **770.** Relationships between dissolved organic matter and mercury cycling in California ecosystems affected by historic mining. **J.A. Fleck**, C. Alpers, M. Marvin-DiPasquale, G. Aiken

ENVR **771.** Occurrence of micropollutants in the Han River, Seoul, Korea. **M. Kim**, S. Tak, T. Kim, J. Lee, W. Choe, Y. Lee, K. Zoh

ENVR **772.** Light-based technology for surface disinfection. N. Wong, N. Zhan, **Q. Chang**, J. Kwan, K. Yeung

ENVR **773.** Simplified method for concentrating volatile disinfection byproducts. **K.E. Furst**

ENVR **774.** Biocomposite magnetic coated chitosan beads for removal of estrone products from water systems. **S.M. Ríos-Bonilla**, V. Fernandez-Alos, O. Perales, F. Roman

ENVR **775.** Effect of UV and chlorination-dechlorination tertiary treatment on pharmaceutic loads in Chicago WWTP effluent. **A. Welch**

ENVR **776.** Evaluation of swellable organically modified silica passive samplers in complex matrices. **S. Pitell**, P. Edmiston

ENVR **777.** Study of degradation products derived from hydrocortisone by ozonolysis. **T. Rahman**, T. Siddiquee

ENVR **778.** Elimination of tetrakis (hydroxymethyl) phosphonium chloride from surface water using biochar as an adsorbent. **S.R. Akech**, O.O. Harrison, A. Saha

ENVR **779.** Using waste products of the seafood industry to reduce anthropogenic carbon dioxide emissions. **B. Barnes**, P. Sharma, U. Onuchukwu, V. Volkis

ENVR **780.** Investigation of anti-depressant load reduction in wastewater treatment plant effluent by hypochlorite disinfection. **R.A. Mole**, P. Edmiston

ENVR **781.** Recyclable superparamagnetic adsorbent based on mesoporous carbon for sequestration of radioactive cesium. **S. Husnain**, W. Um, Y. Chang, Y. Chang

ENVR **782.** Magnetite graphene oxide encapsulated in alginate beads for remediation of heavy metals contaminated wastewater. **C.V. Huong**, A.D. Dwivedi, T.T. Le, S. Seo, E. Kim, Y. Chang

ENVR **783.** Comparing removal efficiencies of 1,4-dioxane and arsenite by nZVI-common oxidants system: Persulfate, peroxymonosulfate and hydrogen peroxide. **Y. Kang**, E. Kim, H. Yoon, D. Oh, Y. Chang

ENVR **784.** Impacts of diverse nanoscale zero-valent iron on aquatic and terrestrial organisms: Physicochemcial insight on nanomaterials. **H. Yoon**, M. Pangging, M. Jang, Y. Hwang, Y. Kang, J. Kim, Y. Chang

ENVR **785.** Inhibition and gene expression of wastewater nitrifying enrichments exposed to cyanide. **V. Kapoor**, M. Elk, J. Santo Domingo

ENVR **786.** Extraction chromatography using various thiosemicarbazone ligands for metal complexation and the potential environmental applications. **K. Richards**, E.C. Lisic

ENVR **787.** Decomposition characteristics of model organic contaminants by persulfate/ZVI system. **Y. Kim**, H. Kwon

ENVR **788.** Magnetization of silicotitanate for separation of cesium from aqueous phase using a magnetic separating system. **Y. Kim**, J. Kim, W. Lim, S. Choi, H. Kwon

ENVR **789.** Detection of volatile arsenic-sulfur species in environments of high level of sulfide. **J. Zhang**, **S. Jamison**

ENVR **790.** Chemical changes during anaerobic decomposition of hardwood, softwood, and old newsprint under mesophilic and thermophilic conditions. **F. De la Cruz**

ENVR **791.** Implication of nanomaterial embedded polymer composites in the environment: Decomposition kinetics and nanorelease of environmentally aging CNT composites based of activation energy calculation. **C. Han**, E. Sahle-Demessie, **A. Zhao**, J. Wang

ENVR **792.** Conceptual design of a cyclone separator for the separation and recovery of the immobilized anionic radionuclides using a flow analysis. **T. Park**, Y. Choi

ENVR **793.** Influence of oxygen concentration in aqueous solutions of electrolyte on the process of singlet oxygen generation during electrochemical disinfection of contaminated water. **N. Barashkov**, **T. Sakhno**, I. Irgibayeva

ENVR **794.** Development of an analytical method for the measurement of the metabolites of Organophosphate Flame Retardants (OPFRs) in human urine using liquid chromatography-tandem mass spectrometry. **J. She**

ENVR **795.** Assessment of the interactions of herbicides with manganese dioxide to evaluate its availability as a possible remediation process. **E. Segura**, N. López-Santiago, A. Ceniceros, M.E. Gutierrez Ruiz

ENVR **796.** Adsorption of copper and lead to ZnS nanomaterial. **J. Cantu**, J.G. Parsons

ENVR **797.** Method development for the chromatographic/mass spectrometric detection of arsenic species in sulfidic waters. **A. Harper**, **D. Bolden**, J. Zhang

ENVR **798.** Adsorption of chromium(VI) metal ions via amino modified biochar. **K. Flores**, D.F. Gonzalez, J.G. Parsons

ENVR **799.** Analysis of heavy metal content in the Conasauga, Oostanaula and Coosa Rivers utilizing the PerkinElmer NexION 350D ICP-MS. W. Hudson, C. Fernandes, D. Jones, **K. Zimmermann**

ENVR **800.** Alteration of membrane-adherent biofilm properties by acoustic cavitation. **A.N. Rosi**, I. Mergos, M. Qiu, H. Verweij, P. Mouser, L.K. Weavers

ENVR **801.** Oxidation of 3,5,6-trichloro-2-pyridinol by heat-activated persulfate. **R. Mogharbel**, F.M. Zullo, C. Yestrebsky

ENVR **802.** Reformulation of treatment system for remediation of polychlorinated biphenyls in paint. **A. Almutairi**, C.G. Lewis, K. Duranceau, C. Clausen, C. Yestrebsky

ENVR **803.** Dechlorination of octachlorodibenzofuran by zero valent magnesium in acidified ethanol system. **A. Mogharbel**, **C. Yestrebsky**

ENVR **804.** Wastewater analysis: Challenges and optimization of solid phase extraction methods. **C. Good**, P. Edmiston

Section A

Moscone Center

Hall D

Green Chemistry & the Environment

Cosponsored by CEI

Financially supported by AEESP

A. M. Balu, R. Luque, S. O. Obare, *Organizers*

6:00 - 8:00

ENVR **805.** Withdrawn.

ENVR **806.** Distribution of microplastic pollution in a tributary of the Three Gorges Reservoir: A case study in Xiangxi River. **K. Zhang**, H. Hu, X. Xiong, C. Wu, P.K. Lam

ENVR **807.** Focal plane array-based micro-FT-IR imaging as an effective tool for microplastic monitoring within wastewater treatment facilities. **A.S. Tagg**, J.P. Harrison, M. Sapp, E.L. Bradley, C. Sinclair, J.J. Ojeda

ENVR **808.** Bioactive compounds in okra seed extract as novel anti-hepatitis C virus agents. **B. Dayal**, K. Basun

ENVR **809.** Microplastic size effect on sorption coefficient and toxicity of polychrinated biphenyl. **R. Jiang**, W. Lin, E. Zeng

ENVR **810.** Relative performance of different peroxone advanced oxidation processes on the Oil Sands Process-Affected Water (OSPW) remediation. **M. Meshref**, A. Singh, M. Belosevic, M. Mohamed Gamal El-Din

ENVR **811.** Fe-assisted hydrothermal liquefaction and sequential catalytic cracking for production of light olefins from protein-rich microalgae. **Y. Hirano**, Y. Arita, Y. Kasai, N. Funakoshi, A. Nishimura, M. Taniguchi, K. Sagata, Y. Kita

ENVR **812.** Nitrogen and sulfur content of natural organic matter. **S. Coleman**, J. Rice

ENVR **813.** Reactions in poly(a-olefin)s: A replacement for alkane solvents. **T. Malinski**, M.L. Harrell, D.E. Bergbreiter

ENVR **814.** Protecting palladium: Balancing stability and reactivity in support-tether design. **D. Paull**, S.P. George

ENVR **815.** Influence of engineered nanoparticles on microorganism growth in the presence and absence of β-lactam antibiotics. **K. Current**, N.M. Dissanayake, S.O. Obare

ENVR **816.** Influence of the engineered iron oxide nanoparticles on the growth and mutagenicity of microorganisms. **N.M. Dissanayake**, K. Current, S.O. Obare

ENVR **817.** Conversion of carbon dioxide to formic acid mediated by light driven electron storage systems. **J.M. Arachchilage**, S.O. Obare

ENVR **818.** Chemical speciation of anthropogenic nanoparticles. **S.O. Obare**

ENVR **819.** Polymers that substantially degrade, decompose or depolymerize: Draft interpretation affecting the notification of new polymers under Canadian new substances notification regulations. **G. Hammond**

ENVR **820.** Extracting calcium and strontium cations from hydraulic fracturing flowback water using pyridine based small molecules. **S.G. Tajc**

ENVR **821.** Withdrawn.

ENVR **822.** Monolithic aerogels of graphene-mixed metal oxides for air purification and disinfection. W. Chen, **Z. Li**, K. Yeung

Section A

Moscone Center

Hall D

Have Great Lakes Restoration Programs Been Successful? The Case of Legacy & Emerging Pollutants

K. C. Hornbuckle, J. J. Pagano, *Organizers*

6:00 - 8:00

ENVR **823.** Pyrogenic carbon materials in facilitating the abiotic degradation of DDT and its metabolites. K. Ding, **W. Xu**

ENVR **824.** Air-Water exchange of legacy and emerging contaminants in Lake Michigan near Chicago. **A. Boesen**, A. Martinez, K.C. Hornbuckle

Section A

Moscone Center

Hall D

Innovative Materials & Technologies for Sustainable Water Purification

Cosponsored by CEI

E. L. Cates, B. P. Chaplin, J. Choe, J. Liu, D. Shuai, W. Zhang, *Organizers*

6:00 - 8:00

ENVR **825.** Effects of biological decontamination on chemical contaminants in emergency drinking water. **E. Brack**, W. Zukas, N. Farhadi, M. McPartlin, T. Tiano

ENVR **826.** Study on new method of TiO_2 nanorod arrays preparation and photocatalytic performance. **G. Wang**, Y. Shih, Y. Su

ENVR **827.** Nanoconfined water in graphene hydrogel as superadsorbents for water purification. **J. Ma**, **Y. Sun**, M. Yang, **M. Zhang**, F. Yu, **F. Yang**, **K. Chu**, J. Zheng

ENVR **828.** Ceria nanoparticles for sustainable heavy metal water filtration application. **M.J. King**, L. MacManus-Spencer, M.E. Hagerman

ENVR **829.** Reversible, selective trapping of perchlorate from water in record capacity by a cationic metal-organic framework. **I. Colinas**

ENVR **830.** Withdrawn

ENVR **831.** Cloning and expression of protocatechuate dioxygenase gene from *Klebsiella pneumoniae*: Application for degradation of sulphonated aromatic amines. **S. Dixit**, S. Garg

ENVR **832.** Preparation and application of substrate-immobilized TiO_2 nano-photocatalysts for organic micropollutants removal. **S. Hong**

ENVR **833.** Properties evolution of fresh nanoscale Zero-Valent Iron (nZVI) in aerobic and anaerobic water. **A. Liu**

ENVR **834.** Synthesis of biochars using household and agricultural byproducts (orange peel, pistachio shells, and corn stover) and their application in lead adsorption from aqueous solutions. **S. Mireles**, H. Rivera, J. Kang, T. Trad, J.G. Parsons

ENVR **835.** Withdrawn.

ENVR **836.** Enhanced photoelectrochemical performance of the TiO_2 nanotube arrays sensitized with Fe_2TiO_5-graphene oxide for glycerol oxidation. **N. Pico**, **M. Niño**, Á. Meléndez

ENVR **837.** Understanding on the effects of pH and organic carbon concentration on nutrients removal in SBR process for treating domestic wastewater. **S. Lee**, M. Park, S. Yeon, D. Park

ENVR **838.** Individual water purification. **W. Zukas**, E. Brack, T. Tiano, J. Dunn, T. Oriard, Z. Gleason, K. Weitz, I. Norris

ENVR **839.** Fundamental study on chromium biosorption by natural biomass. **H. Yang**, D. Park, N. Kim

ENVR **840.** Modeling study of continuous biosorption process for metal removal and recovery by fermentation biowaste. **N. Kim**, J. Seo, H. Yang, D. Park

ENVR **841.** Hydrothermal treatment of sewage sludge to improve biological nitrogen removal process. **M. Park**, S. Lee, S. Yeon, D. Park

ENVR **842.** Optimization of anoxic-oxic process for the treatment of domestic wastewater with low C/N/P ratio. **S. Yeon**, S. Lee, M. Park, D. Park

Section A

Moscone Center
Hall D

Integrated & Sustainable Environmental Remediation

Cosponsored by CEI

S. K. Brar, M. Cledon, R. Galvez, *Organizers*

6:00 - 8:00

ENVR **843.** Comprehensive performance of vermibiofilter on treating typical pollutants. **Y. Wang**, M. Xing

ENVR **844.** Iron stability on the inner surface of PVC-U drinking pipe. **J. Wang**, T. Tao

ENVR **845.** Remediation of *s*-triazine herbicide spills via adsorption and biodegradation using hydrophobic bio-silica particles. **S. Yeom**, J.K. Sakkos, A. Aksan, L.P. Wackett

ENVR **846.** Synthesis and application of chemically-modified solid wastes as filtering devices of antibiotics from wastewater. **B. Sohn**

ENVR **847.** Synthesis and characterization of stabilized oxygen-releasing CaO_2 nanoparticles for soil remediation. **C. Yeh**, W. Chang, R. Wang, Y. Shih

ENVR **848.** Synthesis of magnetic iron oxide nanoparticles for removal reactive black 5: Reaction mechanism. **M. Chang**, Y. Shih

ENVR **849.** Soil organic matter in native prairies and prairie restorations: Structural studies of humic acids with carbon-13 NMR spectroscopy. A.K. Poladi, **J.S. McConnell**

ENVR **850.** Soil organic matter in native prairies and prairie restorations: Humic and fulvic acid fractions. S. Bomma, K. Pallempati, N. Voleti, **J.S. McConnell**

ENVR **851.** Soil organic matter in native prairies and prairie restorations: Organic carbon content. L.R. Morgan, B.M. Mullins, **J.S. McConnell**

ENVR **852.** Distribution of soil phosphorus and nitrate in the Spring Lake watershed region of western Illinois. S. Nicioli, K.E. Ribordy, J. Boeckler, **J.S. McConnell**

ENVR **853.** Metals removal from Acid Mine Drainage (AMD) using Bioelectrochemical System (BES). **J. Liu**, M. Peiravi

ENVR **854.** Removal of oxyanion pollutants via cationic transition metal coordination polymers. **D. Popple**, S. Citrak, K. Tabler-Miller, A. Alvarenga, K. Stone-Hunter, S. Oliver

ENVR **855.** Comparative analysis of compost and alkaline battery oxide amendments for reducing lead solubility and phytoavailability. **N. Abo-Sido**, C. Gallagher, G. Jerz, B. Love, D. Brabander

ENVR **856.** CO_2 Mineralization and utilization by high-gravity carbonation process: Past, present and future. **S. Pan**, M. Wang, S. Pei, Y. Chen, P. Chiang

ENVR **857.** Degradation of textile azo-dyes using enzymatic treatment with soybean peroxidase. **L.G. Cordova Villegas**, N. Biswas, K.E. Taylor

ENVR **858.** Virucidal activity and mechanism of an antimicrobial surface coating. **Q. Chang**, H. Leung, J. Kwan, K. Yeung

Section A

Moscone Center
Hall D

Nanomaterials in Consumer Products: Formulation, Characterization & Applications Across the Product Life Cycle

S. Hussain, A. J. Kennedy, C. Sayes, *Organizers*

6:00 - 8:00

ENVR **859.** Manganese oxide (MnO) nano-powder in microorganism ionizing respirator gen-1 (MIR-1) for personal protection against airborne pathogens. **M. Park**, B. Chua, A. Son

ENVR **860.** Synthesis of nano-structured MoS_2 materials doped with lanthanide element for upconversion enhancement of solar cell performance. **J. Wu**

ENVR **861.** Monitoring released TiO_2 and ZnO nanoparticles in swimming pool. **S. Lee**, S. Jang, Y. Yim, S.I. Yang

ENVR **862.** Withdrawn

ENVR **863.** Fate and transport of nanoscale zinc oxide in subsurface environment. **S.R. Kanel**, S.R. Al-Abed

Section A

Moscone Center
Hall D

New Challenges in Environmental Chemistry: Marine Ecosystems & Microplastics

A. Kahl, *Organizer*

6:00 - 8:00

ENVR **864.** World oceans under serious threat: Debris polystyrene generate styrene oligomer in ocean water and sand areas. M. Okada, **K. Koizumi**, K. Yamada, B. Kwon, K. Saitoh, T. Takemura, N. Maximenko, **K. Saido**, T. Hiaki

Section A

Moscone Center
Hall D

Novel Membrane Materials & Processes for Water Purification

D. Jassby, B. Mi, *Organizers*

6:00 - 8:00

ENVR **865.** Novel membranes for sea water desalination via membrane distillation. **S. Ragunath**, S. Roy, S. Mitra

ENVR **866.** Surface modification of reverse osmosis membrane by graphene oxide grafting with different oxidation degrees. **W.H. Mak**, D. Jun, B. McVerry, M. Kowal, X.W. Huang, R.B. Kaner

ENVR **867.** Advanced membranes enabled by atomic layer deposition. **Y. Wang**

ENVR **868.** Examining relationship of surface chemistry to silica scaling and combined silica-foulant fouling with modified RO membranes. **A. Quay**, T. Tong, M. Elimelech

Section A

Moscone Center
Hall D

Pesticides in Surface Water: Monitoring, Modeling, Mitigation, Risk Assessment & Regulation

J. Gan, K. S. Goh, Y. Luo, D. Young, *Organizers*

6:00 - 8:00

ENVR **869.** Flow-weighted sampling to measure efficacy of a constructed water quality treatment pond in Folsom, CA. **M. Ensminger**, L.R. Oki, S. Teh, J. Sisneroz, B. Pitton, L. Deanovic, M. Stillway, K.S. Goh

ENVR **870.** Development of a California-based receiving waterbody model for pesticide registration evaluation. **Y. Xie**, Y. Luo, N. Singhasemanon, K.S. Goh

ENVR **871.** Aquatic risk evaluation of new pesticide products as part of California pesticide registration – a preventive approach for surface water protection. **N. Singhasemanon**, Y. Luo, X. Deng

ENVR **872.** Protecting surface water from pesticide contamination in California. **K.S. Goh**

ENVR **873.** Analyses of surface water monitoring results for pesticides in agricultural areas of central coast and Southern California. **X. Deng**, D. Wang, K. Kelley, K.S. Goh

ENVR **874.** Pesticide mitigation using woodchip bioreactors in agricultural regions of California. **S.D. Wagner**, X. Deng, G. Bates, P. Krone-Davis, R. Clark, J. Adelaars, K.S. Goh

ENVR **875.** Integrated vegetated ditch system reduces chlorpyrifos loading in agricultural runoff. **B. Phillips**

ENVR **876.** Developing passive sampling methods for bioavailable current-used pesticides in sediment. **W. Lao**, G. Kim, K.A. Maruya

ENVR **877.** Effectiveness of California's surface water regulations at lowering pyrethroid concentrations in surface waters. **R. Budd**, D. Wang, M. Ensminger

ENVR **878.** Towards a spatio-temporal analysis of pesticide concentrations. S. Jiao, O. Sonmez, **D. long**

ENVR **879.** Analysis of 3 commercial tampon brands for presence of herbicide glyphosate. **A. Corcoran**, **A. Hernandez**, **S. Koenig**

Section A

Moscone Center
Hall D

Poly- & Per-Fluoroalkyl Substances: Where, What, When, Why, Who & How

K. Chu, L. S. Lee, J. Liu, V. Yingling, *Organizers*

6:00 - 8:00

ENVR **880.** Systematic investigation of the effects of perfluoroalkyl acid chain length and ionic head group on human serum albumin binding. **J. Ulrich**, A. Glaser, L. MacManus-Spencer

ENVR **881.** Perfluorohexanoic acid pharmacokinetics in mouse, rat, microminipig, pig, monkey and human. **R.C. Buck**, S.A. Gannon

ENVR **882.** Short-chain fluorotelomer-based substances – Common biodegradation pathways. **R.C. Buck**

Section A

Moscone Center
Hall D

Science & Perception of Climate Change

Cosponsored by CEI and CHED

Financially supported by AEESP

S. O. Obare, E. Schoffers, *Organizers*

6:00 - 8:00

ENVR **883.** Economic analysis of the refinery CO_2-Urea-DMC industrial chain. **Y. Han**, **Q. Jiang**, **Z. Song**

ENVR **884.** Novel approaches of environmental effects to reduce the climate change on macroeconomic energy consumption for green marketing. **G. Ren**, E.J. Parish, H. Honda, S. Lee

ENVR **885.** Tackling drought with climate engineering. **H. Gokturk**

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Section A

Moscone Center
Hall D

Sulfidation of Metal-Based Engineered & Natural Nanomaterials: Implications for Their Fate & Effects in the Environment

Y. Bi, D. Fan, P. G. Tratnyek, P. K. Westerhoff, *Organizers*

6:00 - 8:00

ENVR **886.** Fe^0- and sulfidized Fe^0-activated persulfate in oxidative degradation of benzoic acid: A comparative study. **C. Lee**, M. Rayaroth, Y. Chang, Y. Chang

ENVR **887.** Withdrawn.

ENVR **888.** Controlled evaluation of surface coating effects on silver nanoparticle dissolution. **C. Liu**, W. Leng, P.J. Vikesland

ENVR **889.** *In situ* chemical reduction with Z-loy micrometal ZVI and sulfide and bioaugmentation cultures. **J. Freim**, M. Lee, J. Harvey, D. Raymond

ENVR **890.** Effect of $NaBH_4$ on catalytic reduction of p-nitrophenol by nanoscale zerovalent iron. **S. Bae**, S. Gim, H. Kim, K. Hanna

ENVR **891.** Preliminary study on wettability alternation of surface of carbonate rocks using SiO_2 nanofluids. **D. Wang**

ENVR **892.** Material and reactivity characterization of iron sulfides and sulfidated zerovalent iron during reductive dechlorination. **Y. Lan**, E.C. Butler, **P.G. Tratnyek**

ENVR **893.** Abiotic transformation of hexabromocyclododecane by sulfidated nanoscale zerovalent iron: Kinetics, mechanism and influencing factors. **D. Li**, Y. Zhong, W. Huang, P. Peng

ENVR **894.** Effect of aging on reactivity and surface chemistry of sulfidated nanoscale zerovalent iron. **S. Ghoshal**, S. Rajajayavel

Advances in Treatment Processes for Metals & Metalloids

Sponsored by GEOC, Cosponsored by ENVR

Contaminants Transport, Uptake & Remediation at Contaminated Sites

Sponsored by GEOC, Cosponsored by ENVR

Environmental Challenges & Solutions in Unconventional Oil & Gas Development

Sponsored by GEOC, Cosponsored by ENVR

Mineral-Water Interface Chemistry

Sponsored by GEOC, Cosponsored by COLL and ENVR

THURSDAY MORNING

Section A

Moscone Center
2007

Pesticides in Surface Water: Monitoring, Modeling, Mitigation, Risk Assessment & Regulation

Financially supported by Compliance Services International (CSI)

K. S. Goh, D. Young, *Organizers*

J. Gan, Y. Luo, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **895.** Withdrawn.

8:25 ENVR **896.** Examination of the relative contributions of aqueous and dietary uptake to pyrethroid accumulation in organisms at different aquatic trophic levels. **J. Frew**, J. Giddings

8:45 ENVR **897.** Toxicity of pesticide mixtures in the USGS national water quality network. **M. Shoda**, W.W. Stone

9:05 ENVR **898.** Characterization of sediment chemistry, sediment toxicity and macroinvertebrate communities in wadeable streams of the southeastern United States. **P. Moran**, N. Kemble, L.H. Nowell, I. Waite, C. Ingersoll, P. Van Metre, B.J. Mahler

9:25 ENVR **899.** Electrolytic degradation of pesticides in surface water using an activated carbon-based electrode system. **Y. Li**, W. Mitch

9:45 Intermission.

10:05 ENVR **900.** Urban surface water runoff mitigation of Fipronil and its primary degradation products. L. Greenberg, **Z. Cryder**, J. Richards, M. McGinnis, J. Gan

10:25 ENVR **901.** Environmental fate of double-stranded RNA (dsRNA) biopesticides from RNA interference (RNAi)-based crop protection. **K.M. Parker**, M. Sander

10:45 ENVR **902.** Mechanistic insight into remediation and isomerization of methyl-parathion by mixed metal oxide nanocomposites in aqueous solutions. S. Merlos, K. Nick, C.C. Perry, **M.M. Allard**

11:05 ENVR **903.** Chirality in metolachlor can be used to date grounwater in agricultural settings. **C.P. Rice**, C.J. Hapeman, G. McCarty

11:25 ENVR **904.** Implications of sorption nonlinearity on the environmental fate of penconazole. **D.T. Kuo**

11:45 Concluding Remarks.

Section B

Moscone Center
3008

Advances in Resource Recovery & Conservation in Water Systems

Cosponsored by AGFD, CEI and GEOC

S. Ahuja, L. M. Blaney, T. Boyer, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **905.** Nanowire-modified 3D electrode enabling low-voltage electroporation for water disinfection. **Z. Huo**, H. Hu, X. Xie

8:25 ENVR **906.** Synthesis and microstructural characterization of novel manganese oxide coated titanium dioxide ceramic nanofiltration membranes for dye in wastewater filtration. **J.K. Macharia**, J. He, L. Achola, S.L. Suib

8:45 ENVR **907.** Beneficial reuse of produced water from oil & gas fields. **W. Stringfellow**, M. Camarillo, N. Spycher, P.S. Nico

9:05 ENVR **908.** Anaerobic digestion of renewable materials for biogas production: Experimental stage to the field. **O.O. Adetule**

9:25 ENVR **909.** Microbial fuel cells integrate energy production with nutrient management in municipal wastewater plant sidestreams. **K. Orner**, C. Cools, J. Mihelcic, J.A. Cunningham

9:45 Intermission.

10:05 ENVR **910.** Comparative transcriptomic analysis of lipid producing yeast *Cryptococcus albidus*. **S. Vajpeyi**, K. Chandran

10:25 ENVR **911.** Silver recovery from laundry washwater: Role of regeneration and detergent chemistry. **T. Nawaz**, S. Sengupta

10:45 ENVR **912.** Selective removals of heavy metals (Pb^{2+}, Cu^{2+}, and Cd^{2+}) from wastewater by gelation with alginate for effective metal recovery. **F. Wang**, X. Li

11:05 ENVR **913.** Withdrawn.

11:25 ENVR **914.** Effect of ion composition and electrode properties on electrochemical lithium ion recovery process for application in various source waters. **S. Kim**, J. Yoon

11:45 Concluding Remarks.

Section C

Moscone Center
3002

Contaminants in Urban & Coastal Estuarine Ecosystems

Environmental Processes Affecting Chemical Availability & Toxicity

Cosponsored by AGRO

K. L. Armbrust, P. Saranjampour, R. A. Sutton, *Organizers*, *Presiding*

8:00 ENVR **915.** Multiple stressors in coastal ecosystems: Measuring responses across biological scales and generations in model estuarine organisms. **S. Brander**

8:25 ENVR **916.** Metal oxide nanomaterials in marine and estuarine organisms. **C. Torres**, G.N. Cherr

8:50 ENVR **917.** Photolysis and phototoxicity of dibenzothiophene and 4,6-diethyldibenzothiophene in marine ecosystems. **P. Saranjampour**, E.N. Vebrosky, K.L. Armbrust

9:15 ENVR **918.** Photolytic toxicological impacts of 2,6-dichloro-4-nitroaniline (Dicloran) in varying salinities on *Menidia beryllina* (Inland Silversides). **E.N. Vebrosky**, K.L. Armbrust

9:40 Intermission.

10:00 ENVR **919.** Binding of antibacterial agents at Fe(III) oxyhydroxide surfaces: Experimental study and modeling. **K. Hanna**, R. Marsac, S. Martin, J. Boily

10:25 ENVR **920.** Withdrawn.

10:50 ENVR **921.** Synthesis, occurrence and risk assessment of chlorinated by-products of benzophenone-type UV filters in various aquatic matrices. **M.M. Tsui**, K. Ng, S. Chiu, T. Ma, Y. Ho, T. He, M.H. Lam, R. Kong, P.K. Lam, M.B. Murphy

11:15 ENVR **922.** Physiological and behavioural impacts of Pacific ciguatoxin-1 (P-CTX-1) on marine medaka (*Oryzias melastigma*). **Y. Mak**, J. Li, C. Liu, S. Cheng, P.K. Lam, J. Cheng, L. Chan

Section D

Moscone Center
3004

Novel Membrane Materials & Processes for Water Purification

D. Jassby, B. Mi, *Organizers*, *Presiding*

8:30 ENVR **923.** Structurally and synthetically designed next generation novel polyamides for reverse osmosis application. **A. Roy**

9:00 ENVR **924.** High-performance thin-film composite forward osmosis membranes based on self-assembled amphiphilic block copolymer supporting substrate. **Y. Hu**, X. An

9:20 ENVR **925.** Membrane surface modification by graphene oxide: *In situ* regeneration for ultimate fouling control. **C. Finnerty**, E. Garcia, C. Evans, R. Kaliff, B. Mi

9:40 ENVR **926.** Carbon nanotubes-embedded, high-permeable polyamide thin-film composite membranes for desalination. **H. Lee**, T. Lee, H. Park

10:00 Intermission.

10:20 ENVR **927.** Bacteria inactivation via x-ray-induced UVC radioluminescence: Toward in situ biofouling prevention in membrane modules. T. Johnson, E.A. Rehak, S. Sahu, D. Ladner, **E.L. Cates**

10:50 ENVR **928.** Surface engineering of thin-film composite polyamide membranes with sliver nanoparticles during their fabrication process for providing antibiofouling properties. **Z. Liu**, L. Qi, Y. Hu

11:10 ENVR **929.** Photothermal and hydrophilic functionalization of reverse osmosis membranes for enhanced resistance of mineral scaling, organic, and bio-fouling. **J. Ray**, S. Tadepalli, S. Nergiz, K. Liu, L. You, Y. Tang, S. Singamaneni, Y. Jun

11:30 ENVR **930.** Construction of a novel composite membrane with 3D structure for process intensification of membrane separation. **C. Zhang**, R. Xie, W. Wu, X. Li, Z. Liu, X. Ju, W. Wang, L. Chu

Section E

Moscone Center
3016

Applications of Cheminformatics & Computational Chemistry in Environmental Health

C. Grulke, A. J. Williams, *Organizer, Presiding*

8:00 ENVR **931.** Generation of alternative assessment scores using T.E.S.T. and online data sources. **T. Martin**

8:25 ENVR **932.** Use of chemotypes for profiling and exploring the ToxCast chemical-assay landscape. **A. Richard**, C. Grulke, G. Patlewicz, C. Yang, A.J. Williams

8:50 ENVR **933.** Identification and analysis of substructure fragments for developmental and reproductive toxicity endpoints within the Toxic Substances Control Act universe of chemicals. **D.T. Chang**, K.H. Markey, K. Mayo-Bean, W. Irwin, C. Baier-Anderson, C.J. Brinkerhoff, I. Shah, G. Patlewicz, A. Richard, S. Barone

9:15 ENVR **934.** Ecological Threshold for Toxicological Concern (eco-TTC): Assessing the potential of a new tool for environmental hazard assessment. **A. Beasley**, D.T. Chang, M.G. Barron, S.E. Belanger, J.L. Brill, D. DeZwart, M. Embry, B.A. Farr, M. Halder, A. Kienzler, T.J. Norberg-King, R.R. Otter, H. Sanderson, P. Wilson

9:40 Intermission.

10:00 ENVR **935.** Cheminformatics technologies for chemical risk assessment. **D. Fourches**

10:25 ENVR **936.** Using semi-automated curation workflows to collect, organize, and curate the data and models necessary to support the EPA CompTox chemical dashboard. **C. Grulke**, I. Thillainadarajah, R. Sayre, K. Mansouri, A.J. Williams, A. Richard

10:50 ENVR **937.** Supporting read-across predictions of chemical toxicity using high-throughput text-mining. **N. Baker**, T. Knudsen, A.J. Williams, K. Crofton, G. Patlewicz

11:15 ENVR **938.** New databases and software tools for exposomics and toxicological assessment. **Y. Djoumbou Feunang**, D.S. Wishart

11:40 Panel Discussion.

Section F

Moscone Center
3020

Aquatic Photochemistry

Cosponsored by GEOC

Financially supported by AEESP

V. Lin, K. P. McNeill, *Organizers*

W. Arnold, *Organizer, Presiding*

8:30 ENVR **939.** Biphenyl carboxylic acid probe pair for quantifying photochemically generated hydroxyl radical and excited triplet states in aqueous systems containing dissolved organic matter. **V. Lin**, M. Grandbois, K.P. McNeill

8:50 ENVR **940.** Investigation of the coupled effects of molecular weight and charge transfer interactions on the optical and photochemical properties of dissolved organic matter. **G. McKay**, K.D. Couch, S.P. Mezyk, F.L. Rosario

9:10 ENVR **941.** Fluorescence of humic acids in seawater. **L.T. Stirchak**, D. Donaldson

9:30 ENVR **942.** Photo-production of triplet excited states in effluent organic matter. **M. O'Connor**, K. Zimmerman, D.E. Latch, W. Arnold

9:50 ENVR **943.** Transient absorption-based approach to estimate the photophysical properties of triplet dissolved organic matter. **M. Schmitt**, P.R. Erickson, K.P. McNeill

10:10 Intermission.

10:20 ENVR **944.** Using direct observation of singlet oxygen to determine triplet organic matter rate constants. **K.P. McNeill**, P.R. Erickson

10:40 ENVR **945.** Inhibitory effect of dissolved organic matter on indirect phototransformations of organic contaminants. **S. Canonica**, U. von Gunten

11:00 ENVR **946.** Development of the novel chemical probes for examining the triplet-excited state of organic matters. H. Zhou, L. Lian, S. Yan, **W. Song**

11:20 ENVR **947.** Photochemical exposure of natural organic matter induces humification. **P.G. Hatcher**, D.C. Waggoner, N. DiDinato

11:40 ENVR **948.** Photochemical formation of carbonate radical and its effects on the photo-bleaching of dissolved organic matter. **S. Yan**, W. Song, L. Lian, R. Li, Y. Liu

Section G

Moscone Center
3022

Innovative Materials & Technologies for Sustainable Water Purification

Catalytic

Cosponsored by CEI

E. L. Cates, B. P. Chaplin, J. Choe, D. Shuai, W. Zhang, *Organizers*

J. Liu, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 ENVR **949.** Bioinspired heterogeneous catalyst for perchlorate reduction: Continuous improvements with rational ligand design for the rhenium complex reaction center. **J. Liu**, T.J. Strathmann, M. Han, C. Ren

8:55 ENVR **950.** New-TAML activators: Innovative high-performance, low-cost, biosafety-scrutinized solutions for worldwide reduction of micro-pollutants in water. **T.J. Collins**

9:35 ENVR **951.** Removal of priority hazardous pollutants in municipal sewage effluent to meet environmental quality standards of the European Water Framework Directive using TAML Activators. **R. Kanda**

10:00 Intermission.

10:15 ENVR **952.** Design of longer-lived TAML catalysts. **M.A. DeNardo**

10:35 ENVR **953.** Introducing New-TAML activators for ultra-dilute catalytic oxidation in global water treatment. **G.R. Warner**, A.D. Ryabov, J.A. Taylor, F.S. Vom Saal, T.J. Collins

10:55 ENVR **954.** TAML activators for green oxidative degradation of propranolol: A comparative evaluation. **Y. Somasundar**, A.D. Ryabov, T.J. Collins

11:15 ENVR **955.** Smart catalytic films for water purification. **L. Wright**

11:35 ENVR **956.** Microwave assisted in-situ covalent functionalization of graphene with phenoxo-bridged dinuclear Iron complex: Preparation, characterization and evaluation. **J. Yu**, C.J. Miller, D. Waite

Section H

Moscone Center
3006

Poly- & Per-Fluoroalkyl Substances: Where, What, When, Why, Who & How

K. Chu, L. S. Lee, J. Liu, V. Yingling, *Organizers*, *Presiding*

8:30 ENVR **957.** Fast and ultrasensitive screening of novel fluoroalkylated surfactants in aqueous media: On-line solid phase extraction hyphenated to liquid chromatography high resolution mass spectrometry. **G. Munoz**, S. Vo Duy, M. Desrosiers, J. Liu, S. Sauvé

8:55 ENVR **958.** Extraction and analysis of amphibians for four per/polyfluorinated alkyl acids. **C. de Perre**, L.S. Lee, G. Hoover, M. Chislock, B. Tornabene, S. Guffey, J. Hoverman, M. Sepulveda

9:20 ENVR **959.** Perfluorinated Alkyl Substance (PFAS) cytotoxicity: The differential effects of linear and branched isomers. G. Cantu, Y. Xing, **D. Kempisty**

9:45 ENVR **960.** Investigation and remediation of multiple PFAS source zones at an airport to safeguard an at risk water supply. D. Atkinson, J. Lemon, J. Miles, I. Ross, **E. Houtz**

10:10 Intermission.

10:40 ENVR **961.** Why it matters: Frequency, occurrence, transport, and implications of the 40 classes of recently-discovered per- and polyfluoroalkyl substances in aqueous film-forming foam impacted groundwater. **K.A. Barzen-Hanson**, C.P. Higgins, J.A. Field

11:05 ENVR **962.** When do we need PFASs?: A policy and purchasing strategy for reducing their use. **A. Blum**, T. Bruton, A. Soehl, A. Lindeman

11:30 ENVR **963.** Changing regulatory landscape of Per- and Polyfluoroalkyl Substances (PFAS). **S. Thomas**

11:55 Concluding Remarks.

Section I

Moscone Center
2000

Bioprocesses for Engineered Nanomaterials in Soil-Plant Systems

J. C. White, B. Xing, Y. Yang, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ENVR **964.** Tuning NP properties for optimizing plant uptake and translocation. **G. Lowry**, E. Spielman-Sun, E. Lombi, J.M. Unrine

8:30 ENVR **965.** Withdrawn.

8:55 ENVR **966.** Accumulation and transfer of engineered nanoparticles in terrestrial food chains: Correlating physiological and molecular response. **J.C. White**, B. Xing, O. Parkash, J.L. Gardea-Torresdey

9:15 ENVR **967.** Interaction of CuO nanoparticles with floating plant: Toxicity, distribution and transformation. **J. Zhao**, Z. Wang, B. Xing

9:35 Intermission.

9:55 ENVR **968.** Leguminous crop interactions with engineered nanomaterials in soils. **P. Holden**, Y. Wang, D.C. Bouchard, R.M. Nisbet, J.P. Schimel, J.A. Hernandez, J.L. Gardea-Torresdey

10:20 ENVR **969.** Advances in the metrology for characterizing the uptake, translocation and genotoxicity of engineered nanomaterials in terrestrial plants. **B.C. Nelson**

10:45 ENVR **970.** Examining the impact of copper oxide nanoparticles on carrot and lettuce growth and root hydraulic conductivity. **S.J. Parikh**, A.J. Margenot, M. Dumlao, D. Rippner, R.A. Davis, P.G. Green, J.L. Sutcliffe, A. McElrone

11:10 ENVR **971.** Bioformation of silver nanoparticles by plant root systems as affected by growth conditions. **H. Guo**, B. Xing, L. He

11:30 ENVR **972.** Detection of multi-walled carbon nanotubes uptake by lettuce. **K.K. Das**, Y. You, M. Torres, F. Barrios-Masias, B. Xing, Y. Yang

Environmental Challenges & Solutions in Unconventional Oil & Gas Development

Sponsored by GEOC, Cosponsored by ENVR

Contaminants Transport, Uptake & Remediation at Contaminated Sites

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Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Engineering Operando to Larger Scale: Shaped Catalysts & Process Control

Sponsored by CATL, Cosponsored by ENVR and I&EC

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by COLL and ENVR

THURSDAY AFTERNOON

Section A

Moscone Center
2007

Pesticides in Surface Water: Monitoring, Modeling, Mitigation, Risk Assessment & Regulation

Financially supported by Compliance Services International (CSI)

J. Gan, K. S. Goh, *Organizers*

Y. Luo, D. Young, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR **973.** Modeling spray drift and runoff related inputs of pesticides to receiving water. **X. Zhang**, K.S. Goh

1:25 ENVR **974.** Pesticide uptake into runoff evaluated at the field scale. **D. Young**

1:45 ENVR **975.** Improved modeling approaches for pesticide registration evaluation for surface water protection in California. **Y. Luo**, X. Yina, N. Singhasemanon, X. Deng, K.S. Goh

2:05 ENVR **976.** Why are real-world surface water exposure distributions much lower than US EPA FIFRA Tier II EECs? An evaluation based on pyrethroid insecticides. **P. Hendley**, A.M. Ritter, D.A. Desmarteau, C.M. Holmes, J. Giddings, J. Wirtz, J. Frew

2:25 Intermission.

‡ *Cooperative Cosponsorship*

2:45 ENVR **977.** Daily models of agricultural chemical concentrations and loads in rivers draining the Central Valley, California to the San Francisco Bay-delta estuary: Before and during an extended drought. **J. Domagalski**

3:05 ENVR **978.** Modeling pesticide loadings from the San Joaquin watershed using SWAT. **J. Chen**, M. Zhang

3:25 ENVR **979.** Expedition into the realm of environmental monitoring data: How can we make sense and make use of the information contained in the data? **D. Wang**, J. Teerlink, N. Singhasemanon, K.S. Goh

3:45 ENVR **980.** PURwebGIS: Simplifying a large agro-environmental spatio-temporial dataset for quick assessment and decision making. **C. DeMars**, M. Zhang

4:05 Concluding Remarks.

Section B

Moscone Center
3008

Advances in Resource Recovery & Conservation in Water Systems

Cosponsored by AGFD, CEI and GEOC

S. Ahuja, L. M. Blaney, T. H. Boyer, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR **981.** Linking crystal growth kinetics to quantitative sustainable design of Struvite precipitation systems. **S. Agrawal**, J. Guest, R. Cusick

1:25 ENVR **982.** Recovering high-quality phosphorus- and nitrogen-laden fertilizers from poultry litter. **U. Shashvatt**, J. Benoit, H. Aris, L.M. Blaney

1:45 ENVR **983.** Sustainable struvite control and recovery in wastewater treatment plants using residual biogas. **S. Moore**, L. Ma, V. Karanikola, R.G. Arnold, A.E. Saez, D. Moulis, J. Bish, J. Prevatt

2:05 ENVR **984.** Fate and impact of contaminants of emerging concern during nutrient recovery via ion exchange from synthetic anaerobic effluent. **Y. Tong**, P.J. McNamara, B. Mayer

2:25 Intermission.

2:45 ENVR **985.** Two-stage process for phosphorus extraction and recovery from agricultural waste. **S. Sengupta**, J. Beaudry, U. Shashvatt, L.M. Blaney

3:05 ENVR **986.** Calcium phosphate seed nuclei for selective phosphorus recovery at neutral pH. **D. Kim**, M. Cohen, M. Gu, I. Jeon, Y. Jun

3:25 ENVR **987.** Customizable nutrient products recovered using ion exchange technology. **A. Avila**, P.J. McNamara, B. Mayer

3:45 ENVR **988.** Application of the Donnan membrane principle for sustainable nutrient recovery. U. Shashvatt, **L.M. Blaney**

4:05 ENVR **989.** Coupling of Pd nanoparticles and denitrifying biofilm promotes H_2-based nitrate removal with greater selectivity towards N_2. **C. Zhou**, B.E. Rittmann

4:25 Panel Discussion.

4:55 Concluding Remarks.

Section C

Moscone Center
3002

Contaminants in Urban & Coastal Estuarine Ecosystems

Temporal & Spatial Assessment of Persistent-Bioaccumulative Chemicals in Coastal & Urban Waters

Cosponsored by AGRO

J. Meador, D. Muir, R. A. Sutton, *Organizers*, *Presiding*

1:00 ENVR **990.** Legacy and emerging organic contaminants in urban estuaries: A global perspective. **E. Zeng**, L. Liu

1:30 ENVR **991.** Survey of legacy pollutants in margin sediments of central San Francisco Bay. **D. Yee**, P. Trowbridge, J.A. Davis

1:55 ENVR **992.** Continuous release of PCBs from New Bedford Harbor results in elevated concentrations in the surrounding air. A. Martinez, B. Hadnott, A. Awad, N. Herkert, K. Tomsho, K. Basra, M. Scammell, W. Heiger-Bernays, **K.C. Hornbuckle**

2:20 ENVR **993.** Characterizing the advection of Polychlorinated Biphenyls (PCBs) from the sediments in the Lower Duwamish Waterway Superfund site. **J. Apell**, D. Shull, C. Grimmett, P.M. Gschwend

2:45 Intermission.

3:05 ENVR **994.** Perspectives on environmental monitoring and bioaccumulation of contaminants of emerging concern in urban coastal systems. **B.W. Brooks**, S. Burket, S. Haddad, C. Scott

3:35 ENVR **995.** Application of non-targeted analysis approaches to assess input of organic micropollutants to San Francisco Bay. **L. Ferguson**, K. Overdahl, N. DeStefano, R.A. Sutton, J. Sun

4:00 ENVR **996.** Tracking contaminant trends, spatial patterns, and pathways over 20 years of fish contaminant monitoring in San Francisco Bay. **J. Sun**, J.A. Davis, R. Mayfield

4:25 ENVR **997.** San Francisco Bay area wastewater monitoring reveals previously unidentified pathway for pet spot-on flea treatments to reach estuaries. **K.D. Moran**, R.A. Sutton, A.M. Sadaria, R.U. Halden

Section D

Moscone Center
3004

Novel Membrane Materials & Processes for Water Purification

D. Jassby, B. Mi, *Organizers*, *Presiding*

1:00 ENVR **998.** Facile grafting of zwitterions onto membrane surface to improve antifouling properties for wastewater reuse. **H. Lin**, N. Shahkaramipour, S. Ramanan

1:30 ENVR **999.** Withdrawn.

1:50 ENVR **1000.** Quantifying bacterial adhesion to polymeric membranes by single-cell force spectroscopy. **S. BinAhmed**, A. Hasane, Z. Wang, S. Romero-Vargas Castrillon

2:10 ENVR **1001.** Fouling-resistant ultrafiltration membranes by selective swelling of polystyrene-block-poly(ethylene oxide). **H. Yang**, **Y. Wang**

2:30 Intermission.

2:50 ENVR **1002.** Antifouling properties of molybdenum disulfide and graphene oxide for water filtration. I. Alam, L. Guiney, M. Hersam, **I. Chowdhury**

3:20 ENVR **1003.** Evaluation of photocatalytic membrane fouling by humic acid. **R. Zhu**, A. Diaz, S. Solares, D. Shuai

3:40 ENVR **1004.** Fabrication of micro-filtration membrane to mitigate organic fouling during water treatment. **E. Igbinigun**

4:00 ENVR **1005.** Membrane surface charge and wettability parallel tuning through layer by layer assembly for antifouling. **X. Zhu**, B. Chen

Section E

Moscone Center
3016

Applications of Cheminformatics & Computational Chemistry in Environmental Health

C. Grulke, A. J. Williams, *Organizer, Presiding*

1:00 ENVR **1006.** Estimation of hydrolysis rate constants for carbamates. **J. Patel**, C. Tebes-Stevens, E.J. Weber

1:25 ENVR **1007.** In silico alkaline hydrolysis reaction kinetics of HMX and RDX. **M.K. Shukla**, L. Sviatenko, L. Gorb, D. Leszczynska, J.R. Leszczynski

1:50 ENVR **1008.** Using experimental data and computational chemistry to predict reactive sites of polycyclic aromatic hydrocarbons. **I. Titaley**, D. Walden, O. Ogba, P. Cheong, S.L. Simonich

2:15 ENVR **1009.** What works best for predicting human skin sensitization potential of chemicals: *In vitro* data or *in silico* models? V.M. Alves, S. Capuzzi, E. Muratov, R.C. Braga, T. Thornton, D. Fourches, J. Strickland, N. Kleinstreuer, C.H. Andrade, **A. Tropsha**

2:40 Intermission.

3:00 ENVR **1010.** If it looks like, fits like and binds like a CYP450 ligand is it a CYP450 ligand? A molecular profiling case study using MOE. **M.R. Goldsmith**, C. Williams, D.T. Chang

3:25 ENVR **1011.** Structure-based understanding of binding affinity and mode of estrogen receptor α agonists and antagonists. **S. Lee**, M.G. Barron

3:50 ENVR **1012.** Application of functional use predictions to aid in structure identification of chemicals in house dust. **K. Phillips**, A. McEachran, J. Sobus, K. Isaacs

4:15 ENVR **1013.** OPERA: A QSAR tool for physicochemical properties and environmental fate predictions. **K. Mansouri**, C. Grulke, R. Judson, A.J. Williams

4:40 Panel Discussion.

Section F

Moscone Center
3020

Aquatic Photochemistry

Cosponsored by GEOC

Financially supported by AEESP

W. Arnold, K. P. McNeill, *Organizers*

V. Lin, *Organizer, Presiding*

1:00 ENVR **1014.** Photomineralization of dissolved organic matter in acid mine drainage-impacted waters. C. Yuan, L.K. Weavers, P.G. Hatcher, **Y. Chin**

1:20 ENVR **1015.** Photodegradation of pharmaceuticals in partially nitritated wastewater. **P.I. Hora**, P. Novak, W. Arnold

1:40 ENVR **1016.** Trace metal removal in oxidative treatment systems driven by cathodic H_2O_2 production and UV photolysis. **J.M. Barazesh**, C. Prasse, J. Wenk, D. Sedlak

2:00 ENVR **1017.** Amorphous peroxo-titania as a visible light response photocatalyst for oxidation of organic compounds. **J. Seo**, H. Lee, H. Lee, M. Kim, C. Lee

2:20 ENVR **1018.** Modeling the UV/H_2O_2 oxidation of phenolic compounds in a continuous-flow reactor with reflecting wall. **T. Zhang**, R.G. Arnold, G. Diefenthal, A.E. Saez

2:40 Intermission.

2:50 ENVR **1019.** Aquatic photochemical transformations of thiols with dissolved organic matter. **C. Chu**, D. Stamatelatos, P.R. Erickson, M. Schmitt, K.P. McNeill

3:10 ENVR **1020.** Photochemical damage of extracellular enzymes visualized by holistic proteomics techniques and enzymology. **E. Janssen**, C. Egli

3:30 ENVR **1021.** Direct and indirect photochemical reactions in viral RNA measured with RT-qPCR and mass spectrometry. **Z. Qiao**, K. Wigginton

3:50 ENVR **1022.** Modeling the endogenous sunlight inactivation rates of laboratory strain and wastewater *E. coli* and enterococci using biological weighting functions. **A.I. Silverman**, K.L. Nelson

4:10 ENVR **1023.** Photochemical reactive oxygen species generation and redox transformation of iron by the organic exudate secreted by *Microcystis aeruginosa* in natural waters. K. Wang, **S. Garg**, D. Waite

Section G

Moscone Center
3022

Innovative Materials & Technologies for Sustainable Water Purification

Catalytic & Electrochemical

Cosponsored by CEI

E. L. Cates, B. P. Chaplin, J. Choe, J. Liu, D. Shuai, W. Zhang, *Organizers*

W. Zhang, *Presiding*

1:00 Introductory Remarks.

1:05 ENVR **1024.** Oxidant and disinfection byproduct production of a point-of-use electrochemical water treatment device. **J. Bliss**, D.A. Reckhow

1:25 ENVR **1025.** Classification and quantification of electrochemical oxidants generating electrodes with chlorine generation. **J. Kim**, J. Yoon

1:45 ENVR **1026.** Redox-mediated electrochemical methods for water purification and environmental remediation of nitrosamines and contaminants of emerging concern. **X. Su**, L. Bromberg, K. Tan, T.F. Jamison, L. Padhye, T. Hatton

2:05 ENVR **1027.** Using electrolytic oxidation as pretreatment to improve As(III) removal by reverse osmosis membranes. Y. Hou, **B. Mayer**

2:25 ENVR **1028.** Application of quinoid mediators to develop redox-active flow-electrodes for high-performance capacitive deionization. **J. Ma**, D. He, D. Waite, W. Tang, P. Kovalsky, C. Zhang

2:45 Intermission.

3:00 ENVR **1029.** Highly active palladium nanoparticles for catalytic reduction of *N*-nitrosodimethylamine. **H. Ma**, T. Wu, C. Na

3:20 ENVR **1030.** Natural fiber welding of lignocellulose-supported Pd-based catalysts for water purification. **D.P. Durkin**, T. Ye, E.G. Larson, J. Choi, K.J. Livi, H.C. De Long, P.C. Trulove, H. Fairbrother, L. Haverhals, D. Shuai

3:40 ENVR **1031.** Reduction of waterborne contaminants on graphitic carbon nitride supported Pd-based catalysts. **T. Ye**, D. Shuai

4:00 ENVR **1032.** Catalytic destruction of emerging contaminants by structured palladium-based materials. **X. Min**, Y. Wang

Section I

Moscone Center

2000

Bioprocesses for Engineered Nanomaterials in Soil-Plant Systems

J. C. White, B. Xing, Y. Yang, *Organizers*, *Presiding*

1:00 ENVR **1033.** pH-Dependent surface chemistry of biologically and environmentally relevant ligands on oxide nanoparticles. **V.H. Grassian**

1:25 ENVR **1034.** Withdrawn.

1:50 ENVR **1035.** Effect of humic acid on the remediation of hexabromocyclododecane contaminated soil using an integrated nano-bio system. **Y. Chang**, T.T. Le, H. Yoon, J. Kim

2:15 ENVR **1036.** Three-dimensional surface enhanced Raman spectroscopy evaluation and visualization of gold nanoparticle tansport in a silicon-based micromodel. **M. Chan**, W. Leng, S.L. Walker, P.J. Vikesland

2:35 ENVR **1037.** Biodegradation of multi-walled carbon nanotubes by *Mycobacterium vanbaalenii* PYR-1. **Y. You**, K.K. Das, H. Guo, C. Chang, M. Navas-Moreno, J. Chan, P. Verburg, S.R. Poulson, X. Wang, B. Xing, Y. Yang

2:55 Intermission.

3:10 ENVR **1038.** Assessing the risk of engineered nanomaterials in the environment using the nanoFate model. **A.A. Keller**, K. Garner

3:35 ENVR **1039.** Benefits and risks of agricultural use of carbon-based nanomaterials. **M. Khodakovskaya**

4:00 ENVR **1040.** Impacts of copper oxide nanoparticles on soil enzyme activities across diverse ecosystems. **A.J. Margenot**, S.J. Parikh

4:20 ENVR **1041.** Ecotoxicity of manufactured Al nanophases. **A. Masion**, C. Santaella, L. Shintu

4:40 ENVR **1042.** Determining phytotoxicity of carbon nanotubes in heat and drought stressed crops. **J.T. Jordan**, P. Payton, J.E. Canas-Carrell, D. Tissue

Environmental Challenges & Solutions in Unconventional Oil & Gas Development

Sponsored by GEOC, Cosponsored by ENVR

Contaminants Transport, Uptake & Remediation at Contaminated Sites

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Sponsored by CATL, Cosponsored by ENVR and I&EC

Elucidation of Mechanisms & Kinetics on Surfaces

Sponsored by CATL, Cosponsored by COLL and ENVR

FLUO

Division of Fluorine Chemistry

N. Vasdev, *Program Chair*

SUNDAY MORNING

Section A

Grand Hyatt San Francisco

Conference Theatre

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Antonio Togni

J. T. Welch, *Organizer, Presiding*

G. B. Hammond, *Presiding*

8:00 Introductory Remarks.

8:10 FLUO **1.** Studies on fluoroalkylations and fluorinations. **S.G. Prakash**

8:40 FLUO **2.** Radical asymmetric functionalization of alkenes with Togni reagent. **X. Liu**

9:10 FLUO **3.** Recent advances in hydrogen bond-controlled nucleophilic fluorination. **G.B. Hammond**

9:40 Intermission.

10:00 FLUO **4.** Underappreciated alkaline earth chemistry: Halides and organometallic systems. **H.F. Schaefer**

10:30 FLUO **5.** Reactivity of the neutral hypercloso radical, 1-H-(2-6)F_5-(7-12)-$(CF_3)_6CB_{11}$•. J. Plutnar, Z. Janoušek, A. Wahab, J. Ludvík, **J. Michl**

11:00 FLUO **6.** Organometallic approaches to low global warming automotive refrigerants: Nickel complex-catalyzed production of C_4-hydrofluoroalkenes from C_2-fluoroalkenes and silanes. A.J. Sicard, **R. Baker**

11:30 FLUO **7.** Enantioselective methods for carbon-fluorine bond construction. **D. Toste**

SUNDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Conference Theatre

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Antonio Togni

J. T. Welch, *Organizer*

T. Braun, J. Ichikawa, *Presiding*

1:30 FLUO **8.** Reactions of transition metal and main group fluorides and oxofluorides with trimethylsilyl azide and cyanide. P. Deokar, R.M. Haiges, D.A. Dixon, M. Vasiliu, **K.O. Christe**

2:00 FLUO **9.** Organic and organometallic cations in super acidic solutions. M. Malischewski, **K. Seppelt**

2:30 FLUO **10.** Syntheses of fluorinated cyclopentanone derivatives via regioselective CF_2 insertion using transition metal difluorocarbene complexes. **J. Ichikawa**

3:00 FLUO **11.** Activation of SF_6 at transition metal complexes. **T. Braun**, L. Zámostná, C. Berg

3:30 Intermission.

3:45 FLUO **12.** Chemical transformations with metal complexes of unusual silicon ligands. **T.D. Tilley**

4:15 FLUO **13.** Metal-catalyzed and metal-mediated fluoroalkylation of arenes. **J.F. Hartwig**

4:45 FLUO **14.** Synthesis and coordination properties of asymmetric mixed alkyl/perfluoroalkyl substituted pincer ligands. S. Debnath, T.A. Remick, N. Arulsamy, **D.M. Roddick**

SUNDAY EVENING

Section A

Moscone Center

Hall D

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Antonio Togni

J. T. Welch, *Organizer*

8:00 - 10:00

FLUO **15.** Direct trifluoromethylation from fluoroform with dimsyl-K. **S. Qing**, A.V. Matsnev, G. Lin, C. Liu, Y. Chen, J.S. Thrasher

FLUO **16.** Synthesis and characterization of SF_5-containing fullerene derivatives. **S. Qing**, N.J. DeWeerd, A.V. Matsnev, S.H. Strauss, O.V. Boltalina, J.S. Thrasher

MONDAY MORNING

Section A

Grand Hyatt San Francisco

Conference Theatre

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Antonio Togni

J. T. Welch, *Organizer*

N. Santschi, *Presiding*

8:00 FLUO **17.** Difunctionalization-type electrophilic trifluoromethylation reactions of alkenes. **M. Sodeoka**

8:30 FLUO **18.** Hypervalent iodine mediated fluorinations: Versatile tools for the exploration of novel reactivities. **T. Gulder**, A. Andries-Ulmer, C. Brunner

9:00 FLUO **19.** Modulating the reactivity of hypervalent iodine reagents and carbonyl tethers with the trifluoromethyl group. Y. Li, U. Orcel, **J. Waser**

9:30 FLUO **20.** Catalytic trifluoromethylation fluorination by benziodoxol reagents. **K. Szabo**

9:45 Intermission.

10:15 FLUO **21.** Exploring the amazing electronic structure and reactivity of hypervalent iodine compounds. **H.P. Luethi**

10:45 FLUO **22.** CF_3 radical precursors and their reactions with primary radiolysis products – reversible addition of F_3C• to an aromatic model system. **N. Santschi**, T. Nauser

11:15 FLUO **23. Award Address** (ACS Award for Creative Work in Fluorine Chemistry sponsored by the ACS Division of Fluorine Chemistry). Contributing to organofluorine chemistry as an outsider. **A. Togni**

MONDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Conference Theatre

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Antonio Togni

J. T. Welch, *Organizer*

F. Qing, A. Stuart, *Presiding*

1:30 FLUO **24.** New frontier in fluorine chemistry. **K. Mikami**

2:00 FLUO **25.** Late-stage fluorination for PET imaging. **T. Ritter**

2:30 FLUO **26.** Stereoselective carbonyl fluoroolefinations with fluorinated sulfone and sulfoximine reagents. Y. Zhao, Q. Liu, F. Jiang, **J. Hu**

3:00 FLUO **27.** Silver-mediated oxidative trifluoromethylation and pentafluoroethylation of alcohols: Direct synthesis of alkyl trifluoromethyl (pentafluoroethyl) ethers. **F. Qing**

3:30 Intermission.

3:45 FLUO **28.** News about β-peptides with a glimpse at F-derivatives–research, a magical mystery tour. **D. Seebach**

4:15 FLUO **29.** Intramolecular fluorocyclisations of alkenes with a stable hypervalent fluoroiodane reagent. **A. Stuart**, E.G. Hope, G.C. Geary, M. Urbonaite

4:45 FLUO **30.** Strategic incorporation of fluorine into bioactive compounds for medicinal chemistry and drug discovery. **I. Ojima**

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

J. T. Welch, *Organizer*

8:00 - 10:00

15-16. See previous listings.

‡ *Cooperative Cosponsorship*

48, 50-53. See subsequent listings.

TUESDAY MORNING

Section A

Grand Hyatt San Francisco
Conference Theatre

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Antonio Togni

J. T. Welch, *Organizer*

N. Shibata, *Presiding*

8:00 FLUO **31.** Asymmetric desymmetrization via non-metallic C-F bond activation: Synthesis of 3,5-diaryl-5-fluoromethyl-oxazolidin-2-ones with quaternary carbon center. **N. Shibata**

8:30 FLUO **32.** Perspective on fluoride reactivity. **V. Gouverneur**

9:00 FLUO **33.** Access to heterocycles bearing emergent fluorinated substituents — as FAR as possible! E. Schmitt, F. Aribi, A. Panossian, J. Vors, S. Pazenok, **F.R. Leroux**

9:30 Intermission.

9:45 FLUO **34.** New reagents for difluoromethyl and difluoromethylene transfer. **D.A. Vicic**, P.T. Kaplan, L. Xu

10:15 FLUO **35.** 2-Aryl-2-fluorocyclopropylamines: Synthesis, physicochemical properties and monoamine oxidase inhibitor potencies. **G. Haufe**

10:45 FLUO **36.** Preparative fluoroalkylation via visible light induced electron transfer. **C. Stephenson**

11:15 FLUO **37.** Synthesis of β-SCF_3 α-amino acids and β-SCF_3 amines by nucleophilic trifluoromethylsulfenylation of cyclic sulfamidates. **D. Cahard**

TUESDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Conference Theatre

ACS Award for Creative Work in Fluorine Chemistry: Symposium in honor of Antonio Togni

J. T. Welch, *Organizer*

G. Haufe, *Presiding*

1:30 FLUO **38.** From sulfur to selenium: New reagents for direct trifluoromethylchalcogenation. **T. Billard**

2:00 FLUO **39.** Advance in (trifluoromethyl)dibenzoheterocyclic onium salt chemistry for electrophilic trifluoromethylating agents. **T. Umemoto**

2:30 FLUO **40.** Recent progress in the chemistry of SF_5CX_2- and SF_5N-containing compounds. A.V. Matsnev, S.P. Belina, S. Qing, C.A. Parrish, P. Dudzinski, G. Haufe, **J.S. Thrasher**

3:00 FLUO **41.** Preparation and reactions of aryl tetrafluoro-λ⁶-sulfanyl compounds. Applications in materials science. K. Bonetti, A. Rehm, L. Zhong, **J.T. Welch**

Section A

Grand Hyatt San Francisco
Conference Theatre

General Papers

J. T. Welch, *Organizer*

J. Welch, *Presiding*

3:30 FLUO **42.** Accessing perfluoroalkyl nickel(II), (III), and (IV) complexes bearing a readily attached [C4F8] ligand. **S. Yu**, D.A. Vicic

3:50 FLUO **43.** Synthesis and design of highly fluorinated biopolymers as ^{19}F MRI contrast agents. **W.C. Pomerantz**, S. Kirberger, M. Garwood, B. Weegman

4:10 FLUO **44.** Corannulenes with strong electron-withdrawing groups. A. Haupt, M. Kutter, **D. Lentz**

4:30 FLUO **45.** Mild, low-temperature radiofluorination of α-diazocarbonyl compounds *via* copper-catalyzed H–F insertion. **M.K. Nielsen**, A.G. Doyle

4:50 FLUO **46.** 1,1 and 1,3-difluorination reactions using fuoro-benziodoxol reagent. **N. Ilchenko**, M. Hedberg, B.O. Tasch, K.J. Szabo

5:10 FLUO **47.** Ab initio study on enthalpies of formation for organofluorine compounds. **K.R. Jorgensen**

TUESDAY EVENING

Section A

Moscone Center
Hall D

General Posters

J. T. Welch, *Organizer*

8:00 - 10:00

FLUO **48.** Synthesis of high specific activity 4-[^{18}F]fluorophenylalanine using a new diaryliodonium salt precursor. **B. Hu**, A.L. Vāvere, S.E. Snyder, S.G. DiMagno

FLUO **49.** Control of electrical properties by mixed self-assembled monolayers in a water motion active transducer. **Y. Yang**, J. Park, Y. Kim

FLUO **50.** Synthesis of low-molecular fluorine-containing imidazoles. A.S. Bunev, E.V. Sukhonosova, **S. Naumov**

FLUO **51.** Functionalization of fluoro-substituted imidazoles. A.S. Bunev, S. Naumov, G. Ostapenko, **E.V. Sukhonosova**

FLUO **52.** Fluorination of aryl stannanes using nucleophilic fluoride. **R. Gamache**, C. Waldmann, J. Murphy

FLUO **53.** Analysis on the formation potential of disinfection byproducts in the chlorination of aquatic ciprofloxacin. **H. Guo**, Y. Liu, X. Cheng, T. Ke

GEOC

Division of Geochemistry

A. Ilgen, *Program Chair*

SUNDAY MORNING

Section A

San Francisco Marriott Union Square
Union Square North

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Cosponsored by COLL and ENVR

C. S. Kim, P. A. O'Day, *Organizers*

B. Gilbert, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 GEOC **1.** X-ray absorption spectroscopy studies of sorption reactions at mineral-aqueous solution interfaces. **G.E. Brown**

8:55 GEOC **2.** Withdrawn.

9:15 GEOC **3.** Element speciation in atmospheric nanoparticles and implications for human health and biogeochemical cycling. **P.A. O'Day**, E. Reinoso-Maset, K. Nguyen, V. Leppert, H.J. Forman

9:35 GEOC **4.** Cation effects on the reaction between birnessite and Mn(II). **P. Yang**, Q. Wang, M. Zhu

9:55 GEOC **5.** Cation effects on the adsorption and oxidation of fulvic acid by manganese oxides. **Q. Wang**, P. Yang, M. Zhu

10:15 Intermission.

10:35 GEOC **6.** How does light control the mobility of Ni sorbed on birnessite? **F. Marafatto**, B. Gilbert, J. Pena

10:55 GEOC **7.** Nanoscale iron hydroxides: Unique properties and contaminant scavenging mechanisms (a brief history). **C.S. Kim**

11:15 GEOC **8.** Aggregation, surface structure and characterization of iron oxide nanoparticles: The effect of long term aging in aqueous media. **L. Badakhshanian**, A. Quicksall

11:35 GEOC **9.** Ligand effects on amorphous iron and aluminum hydr(oxide) precipitate characteristics. **S. Yeo**, **T. Stewart**, M. Bartolo, J. Herrboldt, L.E. Katz, D. Lawler

11:55 GEOC **10.** Metal(loid) uptake by mineral surface coatings. **D. Singer**

Section B

San Francisco Marriott Union Square
Union Square South

Pore-Scale Geochemical Processes & the Implications to CO2 Geologic Storage

H. Deng, S. Molins, C. Steefel, *Organizers*, *Presiding*

9:00 Introductory Remarks.

9:05 GEOC **11.** Does enhanced characterization of reactive surface area improve prediction of mineral reaction rates in porous media? **L.E. Beckingham**, C. Steefel, E. Mitnick, A. Swift, M. Voltolini, L. Yang, L. Anovitz, J. Sheets, T. Kneafsey, D. Cole, S. Zhang, G. Landrot, J. Ajo-Franklin, D.J. DePaolo, S. Mito, Z. Xue

9:45 GEOC **12.** DFT calculations of structure and dynamics of CO_2 adsorption on kaolinite and montmorillonite surfaces. **L. Tribe**

10:05 GEOC **13.** Brine–biotite interactions under Geologic CO_2 Sequestration (GCS) conditions: Effects of phosphate. **L. Zhang**, D. Kim, Y. Kim, J. Wan, Y. Jun

10:25 Intermission.

10:45 GEOC **14.** Characterising pore scale mineral heterogeneity and solute transport to model reactive transport for CO2 storage. **S. Krevor**, M. Boon, P. Lai, S. Franchini, B. Niu, A. Al-Menhali, C. Reynolds

11:25 GEOC **15.** Interfacial interactions between cations and biotite under conditions relevant to subsurface CO_2 injection. **Y. Min**, Y. Jun

11:45 GEOC **16.** Molecular dynamics simulation prediction of the solubility of gases (CO_2, CH_4, H_2, noble gases) in nano-confined water. **G. Gadikota**, B. Dazas, I.C. Bourg

12:05 GEOC **17.** Elucidating the mineralogical and transport controls on the evolution of porous media using pore scale simulation. **S. Molins**, D. Trebotich, G.H. Miller, C. Steefel

Section C

San Francisco Marriott Union Square
Savoy

Redox-Driven Environmental Geochemical Reactions for Metals, Major Elements & Organic Pollutants

E. E. Roden, Y. Yang, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **18.** Constraints on the coupled redox cycling of carbon and iron. **S.E. Fendorf**, M. Keiluweit

8:45 GEOC **19.** Reactive oxygen species are ubiquitous along subsurface redox gradients. **P.S. Nico**, X. Yuan, J.A. Davis, D. Dwivedi, K. Williams, A. Bhattacharyya, P. Fox

9:05 GEOC **20.** Biogeochemical controls on the stability of iron-bound soil organic carbon. **S. Dunham-Cheatham**, Q. Zhao, D. Obrist, Y. Yang

9:25 GEOC **21.** Fate of ferrihydrite-bound organic carbon during microbial reduction. **D. Adhikari**, Q. Zhao, K.K. Das, J. Mejia, R. Huang, X. Wang, S.R. Poulson, Y. Tang, E.E. Roden, Y. Yang

9:45 Intermission.

10:00 GEOC **22.** Iron reduction enhances decomposition of occluded organic matter: Evidence from carbon stable isotopes. **S.J. Hall**, W. Huang

10:40 GEOC **23.** Developing a mechanistic understanding of environmentally persistent free radical redox formation in soils at ambient conditions. U.G. Nwosu, **R.L. Cook**

11:00 GEOC **24.** Biosnorkel mechanism–direct extracellular electron transfer by pyrogenic carbon. **T. Sun**, J.J. Guzman, A. Enders, L. Angenent, J. Lehmann

11:20 GEOC **25.** Biogeochemical fate and stability of ferrihydrite-organic compound complexes. **D. Wordofa**, S. Dunham-Cheatham, S.R. Poulson, Y. Yang

11:40 GEOC **26.** Soil organic carbon protection in the presence of iron oxides under aerobic conditions. **S.S. Cronk**, C. Gorski

Section D

San Francisco Marriott Union Square
Sutter 1-3

Structure, Properties & Applications of Minerals with Layered Structure

A. Fernandez-Martinez, N. Garg, B. Ma, C. White, *Organizers*

N. Birkner, R. Shivaramaiah, *Presiding*

9:00 GEOC **27.** Layered double hydroxides and their significant role in geochemical processes. **D.L. Sparks**

9:40 GEOC **28.** Withdrawn.

10:10 GEOC **29.** Structural insights on Ni-Al LDHs using wavelet analysis. **M. Siebecker**, D.L. Sparks

10:30 Intermission.

10:45 GEOC **30.** Withdrawn.

11:25 GEOC **31.** Withdrawn.

11:45 GEOC **32.** Thermochemistry of Layered double hydroxides of Li with Al. **R. Shivaramaiah**, A. Navrotsky, M. Paranthaman, R. Riman, A.M. Anderko, L. Li

Subsurface Technologies for Recovery of Fossil & Geothermal Energy

Sponsored by ENFL, Cosponsored by CATL and GEOC

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

SUNDAY AFTERNOON

Section A

San Francisco Marriott Union Square
Union Square North

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Cosponsored by COLL and ENVR

B. Gilbert, C. S. Kim, *Organizers*

P. A. O'Day, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 GEOC **33.** Environmental surface and interface science at GeoSoilEnviroCARS. **P.J. Eng**, J. Stubbs

1:55 GEOC **34.** Atomic structure of the chalcophanite (001) surface: A window into birnessite mineral growth. **J. Stubbs**, P.J. Eng

2:15 GEOC **35.** Impacts of pH and surface coverage on the response of interfacial water structure to the adsorption of arsenate. **T. Xu**, J.G. Catalano

2:35 GEOC **36.** Mechanisms of Fe(II)-catalyzed goethite recrystallization from stochastic simulation. **K. Rosso**, P. Zarzycki

2:55 GEOC **37.** Isotope-resolved 57-Fe(II) interaction with single Fe(III)-(oxyhydr) oxide crystallites: Unraveling dissolution/recrystallization mechanisms. **S. Taylor**, X. Zhang, J. Liu, B. Arey, D.E. Perea, D.K. Schreiber, J.B. Cliff, T. Wietsma, O. Qafoku, K.M. Rosso

3:15 Intermission.

3:35 GEOC **38.** Surface charge dynamics at the iron oxides/electrolyte interface. **P. Zarzycki**, K.M. Rosso

3:55 GEOC **39.** Arsenopyrite-water interface chemistry: Roles of iron (hydr)oxides in arsenic mobility. **Y. Jun**, C.W. Neil, X. Wu

4:15 GEOC **40.** Effect of solution and solid-phase conditions on the Fe(II)-accelerated transformation of ferrihydrite to crystalline iron oxides. **D. Waite**, R. Collins, A. Jones, D. Boland, W. Xiao, C. Glover

4:35 GEOC **41.** Dominating role of weakly complexing ions at the mineral-water interfaces. **S.C. Myneni**

4:55 GEOC **42.** Cesium adsorption on illite: Characterizing the slow adsorption sites. **V. Amaral**, B. Dazas, I.C. Bourg

Section B

San Francisco Marriott Union Square
Union Square South

Pore-Scale Geochemical Processes & the Implications to CO2 Geologic Storage

H. Deng, S. Molins, C. Steefel, *Organizers*, *Presiding*

1:30 GEOC **43.** Carbonation reactions and their effect on pore distributions in a cement exposed to CO2 for 30+ years. **A.G. Stack**, M. Cheshire, L. Anovitz, W. Carey

2:10 GEOC **44.** Phase and isotopic partitioning behavior of boron in supercritical CO_2 – water systems. **B. Thomas**, T. Phan, J. Gardiner, A. Hakala, C. Lopano

2:30 GEOC **45.** Evidence for difference between precipitation in pores and in bulk solution. **Q. Li**, C. Steefel, Y. Jun

2:50 GEOC **46.** Chemical controls on the fracture propagation rate in calcite. **A. Ilgen**, W. Mook, A. Tigges, C. Chisholm, K. Jungjohann

3:10 Intermission.

3:30 GEOC **47.** Leakage potential of cemented wells from carbon storage reservoirs. **S.A. Carroll**, J. Iyer, P. Roy, H. Mason, W.L. Du Frane, S. Walsh, J. Morris

4:10 GEOC **48.** Coal cleat closure during supercritical CO_2 injection and associated permeability drop: From microscale observation to DEM predictions. **Y. Zhang**, M. Lebedev, Z. Zhang, M. Sarmadivaleh, A. Barifcani, S. Iglauer

4:30 GEOC **49.** Reservoir scale numerical simulation of CO_2 injection into Lower Tuscaloosa formation in Mississippi, USA with experimentally validated modeling parameters. **L. Zhang**, Y. Soong, R. Dilmore

Section C

San Francisco Marriott Union Square
Savoy

Redox-Driven Environmental Geochemical Reactions for Metals, Major Elements & Organic Pollutants

E. E. Roden, Y. Yang, *Organizers*

S. Dunham-Cheatham, W. Xu, *Presiding*

1:30 GEOC **50.** Linking carbon stability to iron redox reactions. D. Adhikari, Q. Zhao, K.K. Das, S. Xu, J. Mejia, R. Huang, X. Wang, S.R. Poulson, Y. Tang, D. Obrist, E.E. Roden, **Y. Yang**

2:10 GEOC **51.** Geochemical and genomic analysis of coupled redox transformations of humic substances and iron oxides. **J. Mejia**, N. Stern, S. He, Y. Yang, E.E. Roden, M.A. Ginder-Vogel

2:30 GEOC **52.** Effects of ammonia and variable redox conditions on mineral dissolution. **S. Di Pietro**, H. Emerson, Y. Katsenovich, J.E. Szecsody

2:50 GEOC **53.** Organic matter transformations in wet tropical soils: The effects of redox fluctuation. **A. Bhattacharyya**, A. Campbell, Y. Lin, P.S. Nico, W. Silver, J. Pett-Ridge

3:10 GEOC **54.** Coupled dynamics of iron and iron-bound organic carbon in forest soils during anaerobic reduction. **Q. Zhao**, D. Adhikari, R. Huang, A. Patel, X. Wang, Y. Tang, D. Obrist, E.E. Roden, Y. Yang

3:40 Intermission.

3:50 GEOC **55.** Contaminant dynamics in waters and sediments of acidic pit lakes. **W.D. Burgos**, J. Sánchez-España, I. Yusta

4:30 GEOC **56.** Reducing sugar content in microbial Extracellular Polymeric Substances (EPS) plays a previously unrecognized role in abiotic reduction of environmentally concerned chemicals. F. Kang, X. Zhou, **D. Zhu**

4:50 GEOC **57.** Redox properties of black carbon in promoting the abiotic transformation of organic pollutants. **W. Xu**, K. Ding

5:10 GEOC **58.** Revisiting reduction of PCE and TCE by magnetite. **J.D. Culpepper**, D. Latta, D.M. Cwiertny, M. Scherer

Section D

San Francisco Marriott Union Square
Sutter 1-3

Structure, Properties & Applications of Minerals with Layered Structure

A. Fernandez-Martinez, N. Garg, B. Ma, C. White, *Organizers*

N. Birkner, R. Shivaramaiah, *Presiding*

1:30 GEOC **59.** Crystal structures of defective lamellar compounds and their X-ray identification: Insights into mineral reactions and material reactivity. **B. Lanson**

2:10 GEOC **60.** Manipulating the layered phases in low-CO_2 cements and related minerals. **C. White**, O. Ozcelik, N. Garg

2:40 GEOC **61.** Connecting the microstructure and structure in clay minerals on heating to 1150 °C using in-operando multi-scale X-ray scattering techniques. **G. Gadikota**, A. Allen, F. Zhang

3:00 Intermission.

3:15 GEOC **62.** Rare earth recovery from phosphate fertilizer production waste. **Z. Hu**, A. Eslamimanesh, R. Shivaramaiah, P. Antonick, R. Riman, A.M. Anderko, A. Navrotsky, D. DePaoli, J. Zhang

3:45 GEOC **63.** Withdrawn.

4:15 GEOC **64.** How soluble Mn(III)-pyrophosphate affects the formation of layered birnessite nanosheets by photochemically-assisted Mn oxidation? **H. Jung**, Y. Jun

4:35 GEOC **65.** Effects of Zn presence on the structure and reductive transformation of birnessite. **S. Zhao**, Y. Tang

Computations for CO_2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY MORNING

Section A

San Francisco Marriott Union Square
Union Square North

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Cosponsored by COLL and ENVR

B. Gilbert, P. A. O'Day, *Organizers*

C. S. Kim, *Organizer, Presiding*

8:00 GEOC **66.** Modeling mineral-water interface structure. **J.D. Kubicki**

8:20 GEOC **67.** Development of rare events simulation tools to probe mineral surface reactivity. **A. Wallace**

8:40 GEOC **68.** Water structure and dynamics at the hematite (1-102) surface. **M.E. McBriarty**, G.F. von Rudorff, J. Stubbs, P.J. Eng, J. Blumberger, K.M. Rosso

9:00 GEOC **69.** Water structure and dynamics at the aqueous interface of ferrihydrite nanoparticles. **C. Johnston**

9:20 GEOC **70.** Capturing the ultrafast vibrational decoherence of water at mineral interfaces. A. Boulesbaa, **E. Borguet**

9:40 Intermission.

10:00 GEOC **71.** Tracking site-specific reactions at mineral surfaces. **J. Boily**

10:20 GEOC **72.** NMR at mineral interfaces: Chemical structure, speciation, dynamics, and reactivity. **K.T. Mueller**, N. Washton, J. Fagan

10:40 GEOC **73.** Molecular-scale imaging of gibbsite nucleation at the mica-water interface using *in situ atomic force microscopy*. **B. Legg**, J.J. De Yoreo

11:00 GEOC **74.** Mineral precipitation at mineral-water interfaces. **A. Fernandez-Martinez**, A. Koishi, Y. Hu, Y. Jun, G.A. Waychunas

11:20 GEOC **75.** Understanding phosphate and silicate adsorption, precipitation and polymerization on mineral surfaces using differential pair distribution function analysis. **M. Zhu**, X. Wang

11:40 GEOC **76.** Mineral-water interface studies: Quo vadis? **G.A. Waychunas**

Section B

San Francisco Marriott Union Square
Union Square South

Advances in Treatment Processes for Metals & Metalloids

Cosponsored by ENVR

K. Campbell-Hay, C. F. Wildman, *Organizers*

K. M. Campbell, C. Wildman, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **77.** Biogeochemical investigations of mine water attenuation in lignocellulose-based sulfate reducing bioreactors. **J. Sharp**, D. Drennan, R. Almstrand, L. Lee, L. Figueroa, I. Lee, J. Ladderud, S. Webb

8:35 GEOC **78.** Novel approaches for the selective capture of transition metals from mine waters using low pH sulfur- and sulfate-reducing bioreactors. R. Holanda, A.L. Santos, **B. Johnson**

8:55 GEOC **79.** Bioreactors for the treatment of hexavalent chromium at remote locations in South Africa. **M.F. Deflaun**, M. Erasmus, E. van Heerden

‡ *Cooperative Cosponsorship*

9:25 GEOC **80.** Role of reduced chromium-organic complexes in performance of an *ex situ* bioreactor to remove hexavalent chromium. **C.F. Wildman**, M. Davidson, B. Marvin

9:45 GEOC **81.** Treatment of uranium in groundwater with soluble phosphate: Successes and challenges at the field-scale. **M. Hay**, J. Gillow, P. Moran

10:05 Intermission.

10:25 GEOC **82.** Iron electrocoagulation for removal of dissolved selenium: Impact of oxygen level and pH. **Y. Bae**, N.M. Crompton, J.G. Catalano, D. Giammar

10:45 GEOC **83.** Stabilization of metalliferous mine tailings during mesocosm-scale phytostabilization. **R.A. Root**, R. Maier, J.D. Chorover

11:05 GEOC **84.** Withdrawn.

11:25 GEOC **85.** Design and optimization of constructed wetlands for metal and metalloid treatment at the Minto Mine, in the Yukon, Canada. **M. Haakensen**, V. Friesen, R. Herbert

11:55 Concluding Remarks.

Section C

San Francisco Marriott Union Square
Savoy

Redox-Driven Environmental Geochemical Reactions for Metals, Major Elements & Organic Pollutants

E. E. Roden, Y. Yang, *Organizers*

A. Kappler, K. Weber, *Presiding*

8:00 GEOC **86.** New light shed on important Earth-relevant redox reactions observed at the nanoscale. **M.F. Hochella**

8:40 GEOC **87.** Effect of Fe-metabolizing microbes and humic substances on Cr-immobilization by biogenic and abiogenic magnetite. **A. Kappler**, K. Adaktylos-Surber, A. Sundman, J. Byrne

9:00 GEOC **88.** Structural transformations of manganese oxides by small organic acids and the fate of trace metals. **E. Flynn**, J.G. Catalano

9:20 GEOC **89.** Mineralogical transformation of MnO_2 during redox reactions with organic contaminants. **S.J. Balgooyen**, C.K. Remucal, M.A. Ginder-Vogel

9:40 GEOC **90.** Nitrate photolysis drives fast abiotic oxidation of Mn^{2+}(aq) to Mn(IV) and promotes the formation of δ–MnO_2 nanosheets. **H. Jung**, Y. Jun

10:00 Intermission.

10:20 GEOC **91.** Nitrogen mediated metal redox cycling. **K.A. Weber**, O. Healy, W. Yang, W. Silver

11:00 GEOC **92.** Using time-resolved X-ray absoprtion spectroscopy to probe the mechanism of contaminant oxidation by δ-MnO_2. **Y. Wang**, S. Benkaddour, F. Marafatto, J. Pena

11:20 GEOC **93.** Rates and products of MnO_2 oxidation of Cr(III)-containing iron oxides. **C. Pan**, A. Qian, H. Liu, J. Catalano, D. Giammar

11:40 GEOC **94.** Investigating the role of sediment manganese oxides as a potential predictor for future arsenic contamination of groundwater. **E. Gillispie**, M. Polizzotto, M.C. Jones

Section D

San Francisco Marriott Union Square
Sutter 1-3

Formation, Structure & Reactivity of Biogenic Minerals

O. Duckworth, J. Pena, M. Polizzotto, C. Santelli, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **95.** Endolithic microbial communities from Mona Island (PR), touring of a geochemical paradox on various carbonate mineral substrates. **E. Couradeau**, D.W. Roush, B.S. Guida, F. Garcia-Pichel

8:35 GEOC **96.** Elucidating the structural diversity of bacteriogenic iron oxides formed in circumneutral environments. **A.H. Whitaker**, O. Duckworth, F.M. Michel, D. Peak

8:55 GEOC **97.** Biologically-driven schwertmannite precipitation in acid mine drainage pipelines: Trace metal implications. **K.M. Campbell**, C. Alpers, D. Nordstrom

9:25 GEOC **98.** Sorption of arsenic to biogenic iron (oxyhydr)oxides produced in circumneutral environments. **T. Sowers**, J.M. Harrington, A.H. Whitaker, M. Polizzotto, O. Duckworth

9:45 GEOC **99.** Iron biomineral formation by Fe(II)-oxidizing bacteria. **A. Kappler**, J. Byrne

10:15 Intermission.

10:35 GEOC **100.** Quantifying mycogenic manganese oxide reactivity through chemical and electrochemical measurements. **B. Uster**, E. Mitchel, M.Y. Andrews, R.L. Diaz, L.A. Sombers, O.W. Duckworth

10:55 GEOC **101.** Atomistic perspectives on cation complexes, octahedral vacancies, and the interlayer water of phyllomanganates through molecular dynamics simulations. **A.G. Newton**, K. Kwon

11:15 GEOC **102.** Organo-mineral interactions in *Pseudomonas putida-birnessite composites: Implications for biogenic mineral reactivity*. **J. Pena**, A. Simanova, A. Kroll

11:35 GEOC **103.** Crystal structure and growth of ZnS nanoparticles formed via comparative biological and abiotic pathways. **J. Xu**, M. Murayama, C. Roco, H. Veeramani, M.F. Hochella

11:55 GEOC **104.** Elemental sulfur biomineralization by phototrophs and chemolithotrophs: Model isolate and field studies. **C. Chan**, P.A. Henri, C.L. Marnocha, A. Levy, T.E. Hanson, A. Steele, J.L. Macalady

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

MONDAY AFTERNOON

Section A

San Francisco Marriott Union Square
Union Square North/South

2017 Geochemistry Division Medal Symposium

S. N. Kerisit, *Organizer, Presiding*

A. Ilgen, *Presiding*

1:00 Introductory Remarks.

1:15 GEOC **105.** Phase transitions in layered Mn oxides: Implications for electron storage and transport in soils. **P.J. Heaney**, F.T. Ling, K. Kong, J. Post

1:55 GEOC **106.** Biogeochemical transformation of metal(loid)s in a disturbed critical zone. **J.D. Chorover**, R. Root, C. Hammond, R. Maier

2:35 GEOC **107.** Probing chemical and porosity changes at the bedrock saprolite interface. **A. Sitchler**, S.L. Brantley

3:15 Intermission.

3:35 GEOC **108.** Lessons learned about using data to understand water issues related to shale gas development in Pennsylvania: From science to sociology. **R.D. Vidic**, S. Brantley, D. Yoxtheimer, J. Pollak, K. Brasier

4:15 GEOC **109.** Exploring the subsurface chemical landscapes where water and biota turn rock into soil. **S.L. Brantley**

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Computations for CO2 Capture, Conversion & Sequestration

Sponsored by ENFL, Cosponsored by CATL, COMP, GEOC and MPPG‡

Undergraduate Research Posters

Geochemistry

Sponsored by CHED, Cosponsored by GEOC and SOCED

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

A. Ilgen, *Organizer*

8:00 - 10:00

21, 31, 43, 73, 103. See previous listings.

129, 135, 157, 188-189, 197, 202, 211, 218, 285-286, 294, 322, 334, 340, 346, 360, 362. See subsequent listings.

TUESDAY MORNING

Section A

San Francisco Marriott Union Square
Union Square North

Mineral-Water Interface Chemistry

Cosponsored by COLL and ENVR

J. Bracco, S. R. Higgins, S. Lee, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **110.** Quartz/aqueous solution interface-a microscopic to macroscopic perspective. **M.L. Machesky**, M.K. Ridley, N. Kabengi, N. Allen

8:35 GEOC **111.** Silica/water interfaces investigated by DFT-MD simulations: Structure and SFG spectroscopy revealed in detail. **M.P. Gaigeot**

8:55 GEOC **112.** Molecular origins of the zeta potential. **M. Predota**, M.L. Machesky, D. Wesolowski

9:25 GEOC **113.** Effect of electrolyte concentration on the stern layer thickness at a charged interface. **M.A. Brown**

9:45 Intermission.

10:00 GEOC **114.** van der Waals wetting forces relevant to geologic carbon sequestration from inelastic x-ray scattering. **B. Gilbert**, P. Perera, P. Schuck, D. Sokaras, I.C. Bourg, T. Tokunaga

10:30 GEOC **115.** Investigating water adsorption on surfaces using ambient-pressure XPS: Effects of humidity on copper and molybdenum oxides. **L. Trotochaud**, A.R. Head, S. Pletincx, O. Karslioglu, A. Waldner, H. Bluhm

10:50 GEOC **116.** Heterogeneous nucleation rate of $Mn(OH)_2$ (s) controls structural match between $Mn(OH)_2$ (s) and quartz substrate. **H. Jung**, Y. Jun

11:20 GEOC **117.** Interaction of bacterial cytochromes and iron oxide minerals. **H. Wang**, A. Johs, L. Liang

11:40 GEOC **118.** MINFIT: A spreadsheet-based tool for parameter estimation in an equilibrium speciation software program. X. Xie, D. Giammar, **Z. Wang**

Section B

San Francisco Marriott Union Square
Union Square South

Microbially-Driven Geochemical Reactions: Kinetics & Communities

D. Jones, J. Sánchez-España, B. M. Tebo, *Organizers*

W. D. Burgos, C. M. Hansel, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **119.** Kinetics and pathways of sulfur reactions linked to O, Fe, and C cycling affecting bioavailability. **G.K. Druschel**, F. Kafantaris, D. Fike, P. Schmitt-Kopplin, S. Dvorski

8:35 GEOC **120.** Effect of climate change on coupled biogeochemistry of sulfur and mercury in organic soils. **B.M. Toner**, O.S. Furman, S. Psarska, A. Krupp, J.L. Gutknecht, S.D. Sebestyen, R.K. Kolka, E.A. Nater

9:05 GEOC **121.** Isotopic and proteomic profiles of sulfate reducers cultivated at steady-state. **W.D. Leavitt**, S. Venceslau, J. Waldbauer, F. Boidi, D. Smith, A.S. Bradley

9:35 Intermission.

9:55 GEOC **122.** Photosynthetic iron oxidation in the phylum chlorobi. **S. Crowe**, K. Thompson, R. Simister, A. Hahn, C. Morgan-Lang, S. Hallam

10:25 GEOC **123.** Geochemical and microbiological controls of oxygen production in cyanobacterial mats. **J.M. Klatt**, M. Medina, S. Grim, D. de Beer, G.J. Dick

10:55 GEOC **124.** Living on the edge: Model photoautotrophs from a Proterozoic ocean analog. **T. Hamilton**, C. Schuler, J. Havig, J. Macalady

11:25 GEOC **125.** Chemo-autotrophic and photo-autotrophic arsenotrophy in western USA soda lakes. **R.S. Oremland**

Section C

San Francisco Marriott Union Square

Savoy

Redox-Driven Environmental Geochemical Reactions for Metals, Major Elements & Organic Pollutants

E. E. Roden, Y. Yang, *Organizers*

M. Ginder-Vogel, A. Thompson, *Presiding*

8:00 GEOC **126.** Iron mineral transformations in organic-rich freshwater flocs induced by Fe(II) and sulfide. L.K. ThomasArrigo, C. Mikutta, **R. Kretzschmar**

8:40 GEOC **127.** Key features of redox-fluctuating systems that influence iron cycling. **A. Thompson**, C. Meile, J. Wilmoth, D. Barcellos, C. Chen, B. Ginn, Y. Tang, C. Hodges

9:20 GEOC **128.** Quantifying the rate and extent of Fe^{2+} catalyzed recrystallization of goethite: A combined experimental and modeling study. **P. Joshi**, M. Fantle, C. Gorski

9:40 GEOC **129.** Production of .OH from oxygenation of Fe^{2+} under near-neutral conditions. **A. Qian**, S. Yuan, D. Giammar

10:00 Intermission.

10:20 GEOC **130.** Bioavailable Fe in nontronite decreases during consecutive Fe redox cycles. **B. Shi**, L. Wu, C.M. Smeaton, P. Van Cappellen

11:00 GEOC **131.** Availability of stored electrons in goethite under oxic conditions. E. Tomaszewski, S. Lee, H. Xu, **M.A. Ginder-Vogel**

11:20 GEOC **132.** Fe(II)-Fe(III) electron transfer in a low Fe clay mineral and its implications for U(VI) reduction. **D. Latta**, A. Neumann, W. Premaratne, M. Boyanov, E.J. O'Loughlin, K.M. Kemner, M. Scherer

11:40 GEOC **133.** Manganese and iron oxide-coated redox bars – tools to delineate soil reducing conditions and study the element sorption behavior in wetland soils. **K. Dorau**, T. Mansfeldt

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Section D

San Francisco Marriott Union Square

Sutter 1-3

2017 Geochemistry Division Medal: Symposium in Honor of Dr. Susan Brantley

S. N. Kerisit, A. Sitchler, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 GEOC **134.** Molecular modeling of multicomponent glass and glass surfaces for nuclear waste glass dissolution and glass-to-metal seals applications. **L.J. Criscenti**

8:55 GEOC **135.** Mineral surface topography related to weathering rate for a 3-D model crystal. **J.Z. Bandstra**

9:15 GEOC **136.** Silicate dissolution: Molecular modeling in the context of experimental and field dissolution and weathering. **J.D. Kubicki**

9:45 GEOC **137.** Atoms to pores concepts for mineral growth and precipitation. **A.G. Stack**

10:15 Intermission.

10:35 GEOC **138.** Lab-Field rate discrepancy revisited. **C. Steefel**

11:05 GEOC **139.** Effects of Na^+ and Ca^{2+} on plagioclase dissolution under high salinity conditions: Implications for subsurface CO_2 injection. **Y. Min**, Y. Jun

11:25 GEOC **140.** Using u-series isotopes to quantify chemical weathering rates on Basse-Terre Island, French Guadeloupe. **L. Ma**

TUESDAY AFTERNOON

Section A

San Francisco Marriott Union Square

Union Square North

Mineral-Water Interface Chemistry

Cosponsored by COLL and ENVR

J. Bracco, S. R. Higgins, S. Lee, *Organizers*, *Presiding*

1:30 GEOC **141.** Insights into mineral-water interface dynamics through coupled stable isotope and spectroscopic investigations. **K. Maher**, J. Nelson

2:00 GEOC **142.** Effects of nano-confinement and crystallinity on Zn isotope fractionation during adsorption onto silica surfaces. **J. Nelson**, L. Wasylenki, J.R. Bargar, G.E. Brown, K. Maher

2:30 GEOC **143.** Effect of interlayer cation size and charge on the intercalation of CO_2 and H_2O into hectorite using computer molecular simulations. **N. Loganathan**, O. Yazaydin, G.M. Bowers, A.G. Kalinichev, J. Kirkpatrick

2:50 GEOC **144.** Reductive immobilization of hexavalent chromium by polysulfide-reduced nontronite. M. Shi, **J. Li**, J.S. Zheng

3:10 GEOC **145.** Real-time observations of Rb^+/Na^+ exchange processes at the muscovite (001) – water interface. **S. Lee**, P. Fenter, K.L. Nagy, N.C. Sturchio

3:30 Intermission.

3:50 GEOC **146.** High resolution AFM imaging of ion adsorption and charge distribution at heterogeneous clay mineral-liquid interfaces. **I. Siretanu**, D. Ebeling, M. Andersson, D. van den Ende, F. Mugele

4:20 GEOC **147.** Impact of surface defects on the surface charge of gibbsite nanoparticles. **A. Klaassen**, F. Liu, D. van den Ende, F. Mugele, I. Siretanu

4:40 GEOC **148.** Aluminum oxyhydroxide-water interfaces: Structure, energetics, and effects of gamma-radiation. **S.N. Kerisit**, M.P. Prange, Z. Shen, E.S. Ilton, X. Zhang, L. Kovarik, K.M. Rosso

5:10 GEOC **149.** Withdrawn.

Section B

San Francisco Marriott Union Square

Union Square South

Microbially-Driven Geochemical Reactions: Kinetics & Communities

D. Jones, J. Sánchez-España, B. M. Tebo, *Organizers*

W. D. Burgos, C. M. Hansel, *Organizers*, *Presiding*

1:30 GEOC **150.** Deconstructing and reconstructing microbial communities that promote the natural attenuation of acidic mine waters. **B. Johnson**

2:00 GEOC **151.** Combined biogeochemical cycling of iron, sulphur, carbon and metal(oid)s (As, Pb, Cu, Zn, Cd, Ni, U, Th) in the water column of acidic pit lakes. **J. Sánchez-España**

2:30 GEOC **152.** Biological sulfide mineral transformations in acidic environments. **I. Sanchez Andrea**

3:00 Intermission.

3:20 GEOC **153.** Metal fluxes across the water-sediment interface in a reservoir affected by acid mine drainage: Reactive transport modeling. **E. Torres**, C. Ayora, A. Nardi, R.M. Couture, B. Shafei, P. Van Cappellen

3:50 GEOC **154.** Metagenomic and genomic characterization of novel organisms associated with sulfide mineral leaching in ore and waste rock from the Duluth Complex, Minnesota. **D. Jones**, E. Roepke, M. Sadowsky, P. Novak, J.V. Bailey

4:20 GEOC **155.** Microbial contributions to pyrrhotite oxidation. **K. Hobart**, D. Jones, J. Feinberg, J.V. Bailey

Section C

San Francisco Marriott Union Square

Savoy

Redox-Driven Environmental Geochemical Reactions for Metals, Major Elements & Organic Pollutants

E. E. Roden, Y. Yang, *Organizers*

J. Mejia, L. Wu, *Presiding*

1:30 GEOC **156.** Electrochemical characterization of minerals and their redox reactions with solutes. **P.G. Tratnyek**, M. Bradley, J.Z. Bandstra, Y. Lan

2:10 GEOC **157.** Geochemical cycling and long-term stability of uranium, nickel and arsenic at the Cluff Lake, Saskatchewan uranium mine. **K. von Gunten**, T. Warchola, M. Donner, W. Hao, M. Cossio, C. Boothman, J. Lloyd, P. Blanchard, T. Siddique, K. Konhauser, D. Alessi

2:30 GEOC **158.** Effect of concentration and time on Pu desorption from goethite. **J. Begg**, M. Zavarin, A. Kersting

2:50 GEOC **159.** Electron transfer pathways facilitating U(VI) reduction by Fe(II) on the hematite (001) surface from first principles. **S. Taylor**, M.C. Marcano, U. Becker, K.M. Rosso

3:10 GEOC **160.** Pu(VI) hydroxamate complex formation at circumneutral pH. **K. Morrison**, M. Zavarin, Y. Jiao, A. Kersting

3:30 Intermission.

3:40 GEOC **161.** Role of secondary mineralization in the competitive inhibition of microbial uranium reduction by iron oxides. K. Belli, **M. Taillefert**

4:20 GEOC **162.** Time-Resolved synchotron x-ray scattering and chemical analysis of redox reactions between aqueous Cr(III) and triclinic Na-birnessite. **K. Kong**, P. Heaney, F.T. Ling, J. Post, J. Stubbs, P.J. Eng

4:50 GEOC **163.** Arsenic release from contaminated sediments is limited by manganese redox buffering in Union Lake, New Jersey. **A. Keimowitz**, B. Mailloux, K.M. Wovkulich, J.S. Harkness, J.M. Ross, S.N. Chillrud

5:10 GEOC **164.** Assessment of the influence of climate change on mercury methylation on a molecular scale with a mechanistic reaction-transport model. **S. Helmrich**, D. Vlassopoulos, P.A. O'Day

Section D

San Francisco Marriott Union Square

Sutter 1-3

2017 Geochemistry Division Medal: Symposium in Honor of Dr. Susan Brantley

S. N. Kerisit, A. Sitchler, *Organizers*, *Presiding*

1:30 GEOC **165.** From a single crater lake to a nation's water resources: Lessons from Susan Brantley about science and life. **G. Rowe Jr**

2:00 GEOC **166.** Calcite and sulfur precipitation due to weathering of granites in temperate climates. **V. Marcon**, X. Gu, H. Kim, S. Brantley

2:20 GEOC **167.** Atomistic-scale evaluation of the fracture toughness of silicates in aqueous environments. **J.M. Rimsza**, R. Jones, L.J. Criscenti

2:40 GEOC **168.** Nanometer to centimeter scale analysis and modeling of pore structures in Earth materials. **D. Cole**, L. Anovitz, G. Rother, A. Swift, X. Gu, S.L. Brantley

3:10 Intermission.

3:30 GEOC **169.** Role of organic matter and pyrite oxidation on deep shale weathering: A comparison of gray shale and black shale. **X. Gu**, S.L. Brantley

3:50 GEOC **170.** Snowmelt controls on concentration-discharge relationships and the balance of oxidative and acid-base weathering fluxes in an alpine catchment, East River, Colorado. **M. Winnick**, R. Carroll, K. Williams, R. Maxwell, W. Dong, K. Maher

4:10 GEOC **171.** Soil weathering as an engine for manganese contamination of well water in the North Carolina Piedmont. **M. Polizzotto**, E. Gillispie, N. Rivera, R. Austin, R. Bolich, O. Duckworth, P. Bradley, A. Amoozegar, D. Hesterberg

‡ *Cooperative Cosponsorship*

4:30 GEOC **172.** Distribution and speciation of phosphorus in a granite weathering profile in a temperate climate. **Z. Zhang**, C. Liu, Z. Zhao, M. Zhu

WEDNESDAY MORNING

Section A

San Francisco Marriott Union Square
Union Square North

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

Cosponsored by COLL, ENVR and NUCL

R. Penn, J. A. Soltis, *Organizers*

M. Conroy, F. N. Smith, *Organizers*, *Presiding*

8:30 GEOC **173.** Mineral growth by nanoparticle aggregation: Calcium phosphate minerals. **F. Michel**, A. Hoeher, O. Borkiewicz, J. Rakovan

9:00 GEOC **174.** Direction-Specific interaction force between nanocrystals. **X. Zhang**, Y. He, M. Sushko, J. Liu, L. Luo, J.J. De Yoreo, S. Mao, C. Wang, K. Rosso

9:20 GEOC **175.** Sulfidization of ferric hydroxides – insights into a dynamic electron transfer process. **S. Peiffer**

9:50 Intermission.

10:10 GEOC **176.** Thermodynamics of nanophase manganese oxides: Sodium, potassium, and calcium birnessite and cryptomelane. **A. Navrotsky**, N. Birkner

10:50 GEOC **177.** Interfacial reactions during Mn biogeochemical cycling: Impact on Mn oxide structures and reactivities towards trace metals. **M.A. Hinkle**, E. Flynn, K.G. Dye, J. Post, C. Santelli, J.G. Catalano

11:20 GEOC **178.** Control of solution metal content on the nanostructure and reactivity of mixed Cu-Zn sulfides formed in low-temperature aqueous systems. **J. Xu**, E. Klemm, M.F. Hochella

11:40 GEOC **179.** Formation, aggregation, and *in situ* dissolution behavior of abiogenically and biogenically produced ZnS nanoparticles. **J.R. Eskelsen**, J. Moon, A.M. Jubb, B.O. Wilkins, M. Chiu, B. Gu, E.M. Pierce

Section B

San Francisco Marriott Union Square
Union Square South

Microbially-Driven Geochemical Reactions: Kinetics & Communities

W. D. Burgos, C. M. Hansel, B. M. Tebo, *Organizers*

D. Jones, J. Sánchez-España, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **180.** Oxidative extracellular electron transfer - rethinking the role of microbes in biogeochemical cycles. **A. Bose**

8:35 GEOC **181.** Microbial metabolite and metabolic byproducts promoted dissolution and transformation of Cr-containing minerals. E. Saad, S. Chen, M. Zhu, C. Hansel, **Y. Tang**

9:05 GEOC **182.** Effect of soluble electron shuttles on Iron(III) reduction, methane production, and microbial community dynamics in wetland sediment microcosms. T. Flynn, M.F. Sladek, Z.D. Jensvold, D.A. Antonopolous, J.C. Koval, C.W. Marshall, K.M. Kemner, **E.J. O'Loughlin**

9:25 GEOC **183.** Evidence for low molecular weight thiols as electron shuttles in dissimilatory iron reduction in natural sediments. **E. Eitel**, M. Taillefert

9:45 Intermission.

10:05 GEOC **184.** Fe(II) oxidation by zetaproteobacteria and friends: Mechanisms and influences on biogeochemical cycles. **C. Chan**, S.M. McAllister, B.K. Chiu, E.K. Field, S. Kato, S.W. Polson

10:35 GEOC **185.** Microbial iron redox metabolism in circumneutral pH environments. **E.E. Roden**

11:05 GEOC **186.** Biodegradation of organic additives in the hydraulic fracturing system: These shale wells aint sterile! **P. Mouser**

11:35 GEOC **187.** Uranium biomineralization by the acid tolerant *Caulobacter crescentus OR37*. **K. Morrison**, M. Zavarin, A. Kersting, Y. Jiao

Section C

San Francisco Marriott Union Square
Savoy

Mineral-Water Interface Chemistry

Cosponsored by COLL and ENVR

J. Bracco, S. R. Higgins, S. Lee, *Organizers*, *Presiding*

8:00 GEOC **188.** Modeling the calcite-water interface: Ion adsorption, ion incorporation and mineral growth. **M. Andersson**, S. Dobberschütz, H. Sakuma, K. Sand, K. Dideriksen, D. Tobler, M. Nielsen, J.J. De Yoreo, J. Rodriguez-Blanco, K. Bechgaard, S. Stipp

8:30 GEOC **189.** Solution-Chemistry control of Mg^{2+}-calcite interaction mechanisms: Implication for biomineralization. **J. Xu**, J. Wang, H. Teng

8:50 GEOC **190.** Solution chemistry of hydroxamic acid adsorption onto bastnäsite and calcite. **A. Wanhala**, A.G. Stack

9:10 GEOC **191.** Role of actinide sorption kinetics in a dolomite/brine system and potential transport from nuclear waste repositories in salt. **T.M. Dittrich**, M.P. Dugas, D.T. Reed

9:30 GEOC **192.** Experimental quantification of kinetic factors in the nucleation rate equation. **Q. Li**, Y. Jun

9:50 Intermission.

10:10 GEOC **193.** Lateral and vertical hydration structure of the barite (001)-water interface: An x-ray reflectivity and molecular dynamics study. **J. Bracco**, S. Lee, P. Fenter, J. Stubbs, P.J. Eng, F. Heberling, A.G. Stack

10:30 GEOC **194.** Fast solvent exchange on a mineral-water interface coupled to process-based mineral precipitation models. **A.G. Stack**, J.M. Borreguero, J. Bracco, S.R. Higgins

11:00 GEOC **195.** Investigation of the effect of varying ionic strength of background electrolytes on barite growth: A hydrothermal atomic force microscopy study. **S. Jindra**, S.R. Higgins, J. Book

11:20 GEOC **196.** In situ nanoscale observations of gypsum dissolution by digital holographic microscopy. **P. Feng**, A. Brand, L. Chen, J. Bullard

Section D

San Francisco Marriott Union Square
Sutter 1-3

2017 Geochemistry Division Medal: Symposium in Honor of Dr. Susan Brantley

S. N. Kerisit, A. Sitchler, *Organizers*, *Presiding*

8:30 GEOC **197.** Interaction of lignin with Fe (II) in the environment leads to the production of humic substances in natural waters, sediments, and soils via Fenton chemistry. **P.G. Hatcher**, S.C. Myneni

9:00 GEOC **198.** Retention of CO_2 and CH_4 in kerogen and its importance in enhanced gas recovery. **L.J. Criscenti**, T.A. Ho, Y. Wang

9:20 GEOC **199.** Effect of sea level rise on the production of organohalogens in coastal wetlands. **D. Schlesinger**, C. Joe-Wong, A.T. Chow, S.C. Myneni

9:40 GEOC **200.** Interactions of snow algae, microorganisms, and minerals in snowpack: Implications for Earth's albedo and potential biosignature formation. **E. Hausrath**, Z. Harrold, A. Murray, O. Tschauner, A. Garcia, C. Barlett, J. Raymond

10:10 Intermission.

10:30 GEOC **201.** Top-down and bottom-up controls on molybdenum isotope dynamics in the critical zone. **J. Pett-Ridge**, E.K. King

10:50 GEOC **202.** Earthcasting solute fluxes and soil development in the critical zone. **P. Sullivan**, Y. Goddéris, J. Schott, Y. Shi, X. Gu, L. Jin, S. Billings, S. Brantley

11:10 GEOC **203.** Understanding inorganic carbon dynamics in natural and human-impacted critical zones. **L. Jin**, A. Ortiz, N. Ogrinc, J. Kaye, L. Ma, E. Hasenmueller, P. Sullivan, S. Brantley

Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOC

WEDNESDAY AFTERNOON

Section A

San Francisco Marriott Union Square
Union Square North

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

Cosponsored by COLL, ENVR and NUCL

M. Conroy, F. N. Smith, *Organizers*

R. Penn, J. A. Soltis, *Organizers*, *Presiding*

1:30 GEOC **204.** Synthetic nanoparticle analogues for studying biological response to airborne particulate matter. **A. Pattammattel**, H. Zhang, H.J. Forman, V. Leppert, P.A. O'Day

1:50 GEOC **205.** Size-dependent mineral nanoparticle surface reactivity in aquifer systems. K.A. Lewis, E.M. Defferari, A.L. Swindle, **A. Elwood Madden**

2:10 GEOC **206.** Characterizing reactivity of iron oxide nanoparticles. **R. Penn**, A.M. Stemig, J.L. Voelz, J.H. Strehlau, C. Johnston, W. Arnold

2:30 GEOC **207.** Caesium-rich micro-particles: A window into the meltdown events at the Fukushima Daiichi Nuclear Power Plant. **S. Utsunomiya**

3:00 Intermission.

3:20 GEOC **208.** Behavior of nanoscale Al (oxy)hydroxide minerals under highly alkaline conditions as a function of metal substitution, surface coordination and solution chemistry. **C. Pearce**, J. Hu, A.R. Felmy, A.E. Clark, X. Zhang, K. Page, H. Wang, A.G. Stack, D. Wesolowski, K. Rosso, S. Clark

3:50 GEOC **209.** Theoretical studies of prenucleation clusters. **S.E. Mason**

4:20 GEOC **210.** Life cycle of Boehmite nano-particles in high level nuclear waste tanks: An electron microscopy study of their growth, aggregation and dissolution. **M. Conroy**, J.A. Soltis, S. Chatterjee, F.N. Smith, E. Ilton, E. Buck

4:40 GEOC **211.** Theoretical study of gibbsite dissolution at high pH. **Z. Shen**, K.M. Rosso, S.N. Kerisit

Section B

San Francisco Marriott Union Square
Union Square South

Microbially-Driven Geochemical Reactions: Kinetics & Communities

W. D. Burgos, C. M. Hansel, B. M. Tebo, *Organizers*

D. Jones, J. Sánchez-España, *Organizers*, *Presiding*

1:30 GEOC **212.** Intricate coupling of carbon, nitrogen and iron redox cycling underlying the biogeochemical dynamics of N_2O. **S.D. Wankel**, C. Buchwald, J. Karolewski, K.C. Grabb, C. Charoenpong, C. Hansel, W. Ziebis

2:00 GEOC **213.** Dualling biominerals? Characterizing simultaneously produced fungal biogenic Mn oxides and Se(0). **C. Rosenfeld**, M.A. Hinkle, B.R. James, C. Santelli

2:30 GEOC **214.** Microbial community profiling of bioreactors for process control and optimization. **M. Haakensen**, V. Friesen

2:50 GEOC **215.** Long-term low dissolved oxygen concentration enriches and shifts nitrifier communities. **G. Liu**, J. Wang

3:10 Intermission.

3:30 GEOC **216.** Activity and phylogenetic diversity of microorganisms in subsurface fluids in the upper ocean crust. **J. Amend**, A. Robador, S. Jungbluth, D. LaRowe

4:00 GEOC **217.** How heterotrophic microorganisms access sedimentary organic matter: A few known knowns, and plenty of known unknowns. **A.D. Steen**

4:30 GEOC **218.** Microbial-driven organic carbon degradation in a tundra soil. **Z. Yang**, B. Gu

Section C

San Francisco Marriott Union Square
Savoy

Structure & Reactivity of Cementitious Materials from Advanced Characterization Techniques

N. Birkner, G. Nagabhushana, R. Shivaramaiah, *Organizers*

A. Fernandez-Martinez, B. Ma, *Presiding*

1:30 Introductory Remarks.

1:35 GEOC **219.** Calcium silicate hydrates. **B. Lothenbach**

2:15 GEOC **220.** Hydration dynamics and morphology of cement pastes with engineered nano additives studied via advanced beamline techniques. **K. Kupwade-Patil**, S. Chin, A.Y. Bumajdad, A. Jamsheer, O. Buyukozturk

2:35 GEOC **221.** Effect of magnesium on the stability of C-S-H. **E. Bernard**, A. Dauzères, I. Pochard, B. Lothenbach

2:55 GEOC **222.** Experimentally Driven Building Block Model for Cementitious Materials. **D.B. Brommer**, F. Martin-Martinez, K. Kupwade-Patil, M.J. Buehler, O. Buyukozturk

3:15 GEOC **223.** Impact of alkalis on the atomic structure of calcium alumino-silicate gels: An x-ray pair distribution function investigation. **N. Garg**, C. White

3:35 Intermission.

3:55 GEOC **224.** Tricalcium silicate hydration in absence and presence of aluminate ions: A step towards a molecular understanding of how the hydration rate of cement depends on its formulation. E. Pustovgar, R.K. Mishra, M. Palacios, T. Matschei, R. Verel, H. Heinz, R.J. Flatt, **J. d'Espinose de Lacaillerie**

4:15 GEOC **225.** Controlling cement hydration through the molecular structure of comb copolymer superplasticizers. **D. Marchon**, P. Juilland, E. Gallucci, L. Frunz, **R.J. Flatt**

4:35 GEOC **226.** Structure and reactivity of Portland cement components and cement blends from solid-state NMR spectroscopy. **J. Skibsted**

4:55 GEOC **227.** Characterization of Portland cement clinker by Electron Backscatter Diffraction (EBSD) analysis in the Scanning Electron Microscope (SEM). **C. Roessler**, B. Moeser, H. Ludwig

5:15 GEOC **228.** Simulations reveal the role of composition into the atomic-level flexibility of bioactive glass cements. K. Tian, G. Chass, **D. Di Tommaso**

Section D

San Francisco Marriott Union Square

Sutter 1-3

General Geochemistry

A. Ilgen, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 GEOC **229.** Investigation of uranium uptake mechanisms by plants from abandoned mine lands in the Southwestern United States. **L. Rodriguez Freire**, E. El Hayek, J.M. Blake, C. DeVore, S. Avasarala, A.M. Ali, M. Spilde, K. Artyushkova, A. Brearley, J.M. Cerrato

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

1:55 GEOC **230.** Plutonium incorporation into goethite and hematite during crystallization from ferrihydrite Plutonium incorporation into goethite and hematite during crystallization from ferrihydrite. **E. Balboni**, **M. Zavarin**, **A. Kersting**

2:15 GEOC **231.** Lead, chromium, and arsenic accumulation associated with naturally accumulating iron–manganese oxide coatings on in-situ stream substrates comparing geothermal and non-geothermal waters. **M. Turpin**, J.M. Blake, A.M. Ali, L. Crossey

2:35 GEOC **232.** Some fish species in offshore Fukushima, Japan have the ability to accumulate a specific nuclide (radioisotope). **H. Katsura**

2:55 GEOC **233.** Metal(loid) release from coal mine spoil during simulated weathering. **S. Morrison**, D. Singer, E. Herndon

3:15 Intermission.

3:35 GEOC **234.** Thermodynamic study of transition metal ion-exchanged zeolites A and Y. **L. Wu**, A. Navrotsky

3:55 GEOC **235.** Transformation of ZnO Nanoparticles (NPs) into Layered Double Hydroxide (LDH) precipitates on nano-γ-Al_2O_3: Implications for the fate of ZnO NPs under Al-enriched environment. **B. Wan**, Y. Tang, R. Huang, X. Feng

4:15 GEOC **236.** Oxygen isotope ratios of phosphate as proxy for polyphosphate cycling in bacteria. **G. Unal Tosun**, Y. Bai, L.M. Stout, D. Jaisi

4:35 GEOC **237.** NMR Correlation spectroscopy of liquids at geochemical pressures. M.P. Augustine, **G. Ochoa**, W.H. Casey

Advances in Resource Recovery & Conservation in Water Systems

Sponsored by ENVR, Cosponsored by AGFD, CEI and GEOC

Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOC

WEDNESDAY EVENING

Section A

Moscone Center

Hall D

2017 Geochemistry Division Medal: Symposium in Honor of Dr. Susan Brantley

S. N. Kerisit, A. Sitchler, *Organizers*

6:00 - 8:00

GEOC **238.** Phosphorus speciation in dust and source soils in the interior American west. **Z. Zhang**, H. Goldstein, R. Reynolds, M. Zhu

Section A

Moscone Center

Hall D

Advances in Treatment Processes for Metals & Metalloids

Cosponsored by ENVR

K. Campbell-Hay, C. F. Wildman, *Organizers*

6:00 - 8:00

GEOC **239.** Biogeochemistry of antimony(V) in microcosms under sulfidogenic conditions. C.R. Johnson, D.A. Antonopolous, M. Boyanov, T. Flynn, J.C. Koval, K.M. Kemner, **E.J. O'Loughlin**

GEOC **240.** Passivation of uranium ore material surfaces with uranyl phosphate precipitation. **T. Kane**, K.M. Campbell, M. Hay

GEOC **241.** Analysis of U(VI) adsorption to biochar using x-ray absorption spectroscopy and isothermal titration calorimetry. **M. Alam**, D. Gorman-Lewis, N. Chen, K. Konhauser, D. Alessi

GEOC **242.** Release of metal(loid)s from coal fly ash and their transformation in aquatic boreal systems. **K.P. Milke**, S.M. Hayes, J.J. Guerard

GEOC **243.** Geopolymer-based solutions for heavy metal waste solidification and stabilization. **M. Lacks**, L.E. Katz, M. Juenger

GEOC **244.** Remediation of heavy metal contaminated soil with coupled soil washing and electro-kinetic field. X. Mao, **F.X. Han**, X. Shao, Z. Arslan, K. Guo

GEOC **245.** Application of biodegradable chelators and vegetable oils in the removal of heavy metals from soils. **M. Sung**, G. Liu, Y. Chen

Section A

Moscone Center

Hall D

Contaminants Transport, Uptake & Remediation at Contaminated Sites

Cosponsored by ENVR

B. H. Jeon, M. B. Kurade, Y. Sik Ok, D. Tsang, *Organizers*

6:00 - 8:00

GEOC **246.** Uncovering the sources of elevated arsenic levels in classic Maya human remains. **C.C. Ivanovich**, E.L. Smith, J. Monge, C. Halperin, B.R. Just, S.C. Myneni

GEOC **247.** World oceans under serious threat: Debris polystyrene in ocean water and sand areas surrounding Japan. **K. Koizumi**, M. Okada, K. Amamiya, K. Takatama, D.M. Karl, H. Katsura, S. Chung, **K. Saido**, T. Hiaki

GEOC **248.** Slow pyrolyzed biochar for Pb and As immobilization, and microbial community abundance of contaminated soils. A. Igalavithana, Y. Xiao, A. El-Naggar, **Y. Sik Ok**

GEOC **249.** Efficacy of acetate-amended biostimulation for uranium sequestration: Combined analysis of sediment/groundwater geochemistry and bacterial community structure. **J. Xu**, H. Veeramani, N. Qafoku, G. Singh, A. Pruden, M.F. Hochella

GEOC **250.** Optimizing magnetite formation for magnetite-based remediation of arsenic groundwater contamination. **A. Yusov**, J. Jamieson, J. Sun, H. Prommer, B.C. Bostick

GEOC **251.** Hydrous zirconium oxide impregnated alginate beads for simultaneous sorption of hexavalent chromium and copper from aqueous solutions. R. Kumar, K. Kim, J. Jang, **B. Jeon**

GEOC **252.** Simulated physical weathering effects on bioaccessibility and speciation of arsenic in mine tailings. **S. Hok**, B. Lamb, N. Burtis, J. Cooper, C. Kim

GEOC **253.** Correlating arsenic bioaccessibility & bioavailability through *in vivo rat exposures*. **T. Oliaro**, B. Lamb, D. Hok, F. Silva, M. Gothong, C. Kim

GEOC **254.** Biodegradation of fluoroquinolone antibiotic from aqueous media by an acclimated green microalgae *Chlorella vulgaris*. **J. Xiong**, S. Saha, H. Kim, B. Jeon

Section A

Moscone Center

Hall D

Environmental Challenges & Solutions in Unconventional Oil & Gas Development

Cosponsored by ENVR

D. Alessi, J. Blotevogel, T. Borch, S. Flynn, *Organizers*

6:00 - 8:00

GEOC **255.** Evaluating changes in groundwater and stream-water chemistry during natural-gas development of Pennsylvania's Marcellus shale. **J. Sohng**, E. Barth-Naftilan, J. Saiers

Section A

Moscone Center

Hall D

Formation, Structure & Reactivity of Biogenic Minerals

O. Duckworth, J. Pena, M. Polizzotto, C. Santelli, *Organizers*

6:00 - 8:00

GEOC **256.** Probing the sorption of metalloids onto synthetic and mycogenic manganese oxides. **C.E. Heath**, B. Uster, O.W. Duckworth

Section A

Moscone Center

Hall D

General Geochemistry

A. Ilgen, *Organizer*

6:00 - 8:00

GEOC **257.** Impact of calcium on the retention and stability of OM in Fe-(Ca)-OM adsorption complexes. **T. Sowers**, J. Stuckey, D. Adhikari, Y. Yang, D.L. Sparks

GEOC **258.** Withdrawn.

GEOC **259.** Using NaCl as a model system to study stable mineral recrystallization. **P. Joshi**, C. Gorski

GEOC **260.** Physiological extractions of metal(loid)s from coal fly ash in interior Alaska. **J. Sterle**, S.M. Hayes, J.J. Guerard

GEOC **261.** Geochemical and hydrologic controls on mercury methylation within an upper-Midwestern terrace fen. **S. Lopez**, A. Graham

GEOC **262.** Molecular investigation of soil organic carbon composition, spatial variability, and depth distribution across a subalpine catchment. **H. Hsu**, C. Lawrence, M. Winnick, J. Druhan, K. Williams, K. Maher

GEOC **263.** Study of heavy metals mobility in acid drainage and its geological interaction in Taxco, Mexico. **T. Rico**, A. Ceniceros, M.E. Gutierrez Ruiz, L. Martínez-Jardines, F. Romero

GEOC **264.** Withdrawn.

GEOC **265.** Spatiotemporal variability in MeHg production in a Restored Oak Savanna Floodplain. **S. Van Helten**, A. Graham

GEOC **266.** Kinetic studies on the spontaneous realumination of hydrothermally treated zeolite Y. **V.A. Mendiola**, S. Crawford

‡ *Cooperative Cosponsorship*

GEOC **267.** Lessons learned from the natural analogue studies relevant to the Korean geological environments of granites and KAERI's disposal research. **T. Park**, M. Baik

GEOC **268.** ^{17}O NMR of the flat aluminum and gallium polyoxocations: Models for minerals. **C. Colla**, C. Fields, A. Oliveri, B. Phillips, W.H. Casey

GEOC **269.** Biogeochemical trace element profiles of urban fruit trees: A resource to increase food security. **H. Oettgen**, C. Gallagher, D. Brabander

GEOC **270.** Kinetic studies of long range metal cation migration through porous zeolitic materials using DRIFT spectroscopy. **E.A. Gorrie**, **S. Nunes**, S. Crawford

GEOC **271.** SFG spectroscopy of Silica/water interfaces by DFT-MD simulations. **S. Pezzotti**

Section A

Moscone Center
Hall D

Microbially-Driven Geochemical Reactions: Kinetics & Communities

W. D. Burgos, C. M. Hansel, D. Jones, J. Sánchez-España, B. M. Tebo, *Organizers*

6:00 - 8:00

272. Microbial communities associated with methylmercury production in two sulfate-impacted northern Minnesota lakes. **D. Jones**, G. Walker, N.W. Johnson, C. Mitchell, J. Coleman Wasik, J.V. Bailey

Section A

Moscone Center
Hall D

Mineral Nucleation: Transient Intermediates & Phase Transitions

B. Legg, S. L. Riechers, *Organizers*

6:00 - 8:00

GEOC **273.** Real-Time and in situ imaging of Akaganéite nanoparticle growth in aquous solution using liquid cell transmission electron microscopy. **F. Wang**, M. Zhu

Section A

Moscone Center
Hall D

Mineral-Water Interface Chemistry

A Tribute to Glenn Waychunas

Cosponsored by COLL and ENVR

B. Gilbert, C. S. Kim, P. A. O'Day, *Organizers*

6:00 - 8:00

GEOC **274.** Adsorption and oxidation of fulvic acid by birnessite under various pH conditions. **Q. Wang**, P. Yang, M. Zhu

GEOC **275.** Investigations of organic ligands with iron oxide mineral/water interfaces using second harmonic and sum frequency generation spectroscopic techiques. **A.L. Mifflin**, K. Michaud, A. O'Neal, D. Antonio

GEOC **276.** Mobility and toxicity of polyoxometalates of W and As, P, and Si. **L. Davidson**, E. Haque, A. Nghiem, B.C. Bostick

GEOC **277.** Reactions of birnessite with Mn(II) under anoxic conditions. **P. Yang**, Q. Wang, M. Zhu

Section A

Moscone Center
Hall D

Mineral-Water Interface Chemistry

Cosponsored by COLL and ENVR

J. Bracco, S. R. Higgins, S. Lee, *Organizers*

6:00 - 8:00

GEOC **278.** Description of the corundum (α–Al_2O_3) – water interface from DFT–MD simulations. **M.K. Ridley**, D. Tunega

GEOC **279.** Adsorption of oxalic acid on rutile surfaces. **D. Biriukov**, **M. Predota**, O. Kroutil, **M.K. Ridley**, **M.L. Machesky**

GEOC **280.** Impact of organic molecules on the colloidal stability of silica nanoparticles – simulations and experiments. **D. Biriukov**, **M. Predota**, O. Kroutil, J.K. Rosenqvist, C.M. Jonsson

GEOC **281.** Fate of trace metals during aluminum oxyhydroxide phase transitions: Implications for reactivity. **F.N. Smith**, D.G. Burtt, S. Chatterjee, M. Conroy, J.A. Soltis, E. Ilton, E. Buck

GEOC **282.** Mapping shale surface charge heterogeneity and surfactant adsorption via atomic force microscopy. **S. Das**, B. Ellis

GEOC **283.** Calcite dissolution rate spectra measured by digital holographic microscopy. **A. Brand**, P. Feng, J.W. Bullard

GEOC **284.** Development of a downhole tool for measuring enthalpy in geothermal reservoirs. **W.C. Corbin**, G. Cieslewski, R.F. Hess, B. Klamm, L. Goldfarb, T.J. Boyle, W.G. Yelton

Section A

Moscone Center
Hall D

Redox-Driven Environmental Geochemical Reactions for Metals, Major Elements & Organic Pollutants

E. E. Roden, Y. Yang, *Organizers*

6:00 - 8:00

GEOC **285.** Ferrihydrite – Carbon dynamics in the presence of Fe(II). **Z. Zhou**, D. Latta, T. Borch, N. Noor, A. Thompson, R. Young, M. Scherer

GEOC **286.** Reductive pathway to Mo deposition in anoxic sediments: Aqueous Mo^{VI} to insoluble Mo^{IV} via variable-composition Fe-Mo^{IV}-S precipitates. **P. Vue**, **A. Vezina**, A. Chappaz, T.P. Vorlicek

GEOC **287.** Redox properties of layer-type manganese oxide minerals. **S. Benkaddour**, F. Marafatto, Y. Wang, M. Sander, J. Pena

GEOC **288.** Formation and reactivity of ferrihydrite-soil organic carbon-calcium ternary complexes. D. Adhikari, T. Sowers, J. Stuckey, D.L. Sparks, **Y. Yang**

GEOC **289.** Electron doping goethite with Fe(II): Influence on goethite properties and reactivity. **L.N. Andrade**, D. Latta, A. Neumann, K. Rosso, M. Scherer

GEOC **290.** Arsenic oxidation by the mighty manganese soils of graskop. **M. Fischel**, C. Dowding, D.L. Sparks

GEOC **291.** Interactions of vanadium(V) with Fe(II)-bearing minerals. **E.J. O'Loughlin**, M. Boyanov, K.M. Kemner

Section A

Moscone Center
Hall D

Structure & Reactivity of Cementitious Materials from Advanced Characterization Techniques

N. Birkner, G. Nagabhushana, R. Shivaramaiah, *Organizers*

6:00 - 8:00

292. Quantifying readily soluble calcium in class C fly ash by Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). **L.N. Perry**, P. Feng, P.E. Stutzman, J. Bullard

Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOC

THURSDAY MORNING

Section A

San Francisco Marriott Union Square
Union Square North

Environmental Challenges & Solutions in Unconventional Oil & Gas Development

Cosponsored by ENVR

D. Alessi, J. Blotevogel, T. Borch, S. Flynn, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **293.** Withdrawn.

8:35 GEOC **294.** Factors controlling the temporal change in chemical composition of Marcellus Shale produced water: Insights from laboratory experiments to field sites. **T. Phan**, A. Hakala

8:50 GEOC **295.** Arsenic mobilization in carbonate-rich shales during hydraulic fracturing. **W. Fan**, K.F. Hayes, B. Ellis

9:10 GEOC **296.** Geochemical modeling of arsenic incorporation during barite precipitation. **F.T. Ling**, H.A. Hunter, J.P. Fitts, A. Lanzirotti, A.S. Acerbo, C.A. Peters

9:25 GEOC **297.** Effects of a phosphonate-based scale inhibitor on brine–biotite interactions: Implications for CO_2-enhanced hydrocarbon recovery. **L. Zhang**, Y. Jun

9:40 Intermission.

10:00 GEOC **298.** Chemical transformations in high volume hydraulic fracturing fluids. **D.L. Plata**, P. Mouser, M. Elsner, B. Drollette, A.J. Sumner

10:20 GEOC **299.** Characterization of a hydraulically fractured well over a one year period: From fracturing fluid to produced water quality. **K. Linden**, J. Rosenblum, E. Thurman, I. Ferrer, G. Aiken

10:40 GEOC **300.** Isolation, analysis, and fingerprinting of organic compounds from hydraulic fracturing fluids using solid phase extraction and liquid chromatography mass spectrometry. **K. Sitterley**, K. Linden, I. Ferrer, E. Thurman

10:55 GEOC **301.** Ion mobility mass spectrometry of hydraulic-fracturing fluids. **E.M. Thurman**, I. Ferrer, J. Zweigenbaum, A. Boice, J. Fjeldsted

11:10 GEOC **302.** Characterization of secondary precipitates in flowback water from hydraulic fracturing and their contribution to zebrafish embryo toxicity. **S. Flynn**, K. von Gunten, Y. He, E. Folkerts, T. Blewett, Y. Zhang, D. Ruan, J.W. Martin, G. Goss, D. Alessi

11:25 GEOC **303.** Assessment of water quality and toxicity downstream of NPDES oil and gas produced water discharges. **M. McLaughlin**, J. Blotevogel, J. Argueso, T. Borch

11:40 GEOC **304.** Biological toxicity associated with lake sediments impacted by oil & gas wastewater disposal. **W.D. Burgos**, L. Castillo-Meza, J. Vanden Heuvel, N. Warner, M. McLaughlin, T. Borch

Section B

San Francisco Marriott Union Square
Union Square South

Contaminants Transport, Uptake & Remediation at Contaminated Sites

Cosponsored by ENVR

M. B. Kurade, D. Tsang, *Organizers*

B. H. Jeon, Y. Sik Ok, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **305.** Removal mechanism for technetium (^{99}Tc) using $Fe(OH)_2$(s) at the Hanford Site, WA, USA. **W. Um**

8:35 GEOC **306.** Recovery of useful resources in shale gas produced water during water treatment. **E. Chung**

9:05 GEOC **307.** Subsurface oil body delineation at a spill site using near-surface temperature gradients. **E. Warren**, B.A. Bekins

9:25 GEOC **308.** Withdrawn.

9:45 Intermission.

10:00 GEOC **309.** Contaminated site remediation by biochars derived from various types of sewage sludge. **D. Tsang**, J. Yoo

10:25 GEOC **310.** Impacts of burning intensity on metal reactivity in wood ash. **A. Rahman**, E. El Hayek, R.J. Bixby, J.M. Blake, A.M. Ali, A.L. Clark, K. Artyushkova, E. Peterson, J.M. Cerrato

10:45 GEOC **311.** Mechanisms of the reductive immobilization of hexavalent chromium by wheat straw biochar. **M. Cossio**, M. Alam, K. von Gunten, J. Kenney, A. Gorzsás, N. Chen, K. Konhauser, D. Alessi

11:05 GEOC **312.** Uranium uptake and redistribution in the transformation of ferrihydrite to goethite. **J.A. Soltis**, E.S. Ilton, O. Qafoku, S. Spurgeon, E. Buck, J.J. De Yoreo

11:25 GEOC **313.** Pentachlorophenol (PCP) removal and dechlorination patterns during oxygen-rich thermal treatment. **J. Davis**, L.E. Katz, H. Liljestrand

11:45 GEOC **314.** Simulation of heavy metal migration in MSWI bottom ash landfill site. **H. Zhang**

Section C

San Francisco Marriott Union Square
Savoy

Structure & Reactivity of Cementitious Materials from Advanced Characterization Techniques

N. Birkner, G. Nagabhushana, R. Shivaramaiah, *Organizers*

N. Garg, C. White, *Presiding*

8:00 Introductory Remarks.

8:05 GEOC **315.** $CaSO_4$ crystallization: From nano-bassanite to mega-gypsum. **A.E. Van Driessche**

8:25 GEOC **316.** Quantifying the dissolution rates of cementitious minerals with *in situ digital holographic microscopy: Tricalcium aluminate and tetracalcium aluminoferrite*. **A. Brand**, P. Feng, J.W. Bullard

8:45 GEOC **317.** Evidence of multiple sorption modes in AFm phases using Mo as structural probe. **B. Ma**, A. Fernandez-Martinez, S. Grangeon, L.L. Charlet

9:05 GEOC **318.** Performance of alkali-activated Turkish Fly Ashes at high temperatures. **C. Meral**

9:25 GEOC **319.** Swelling of Alkali–Silica Reaction (ASR) gels and the resulting damage in concrete. **F. Rajabipour**, A. Gholizadeh

9:45 Intermission.

10:05 GEOC **320.** Accurate determination of hydroxide concentration in activating solutions: New insights into metakaolin reactivity towards geopolymerization. **J. Aupoil**, J. Champenois, J. D'Espinose de Lacaillerie, A. Poulesquen

10:25 GEOC **321.** Effect of temperature and calcium to silicon ratio on structure of calcium (alumino)silicate hydrate at atomic scale and nano scale. **J. Li**, G. Geng, R. Myers, S. Ortaboy, C. Carraro, R. Maboudian, P. Monteiro

10:45 GEOC **322.** Relating the viscoelastic properties of calcium-(alumino)-silicate-hydrate with molecular structure. **P. Mondal**

11:05 GEOC **323.** Intermolecular interactions between nanolayers of calcium-silicatae-hydrates using free energy perturbation method. S. Masoumi, **A. Morshedifar**, M. Abdolhosseini Qomi

11:25 GEOC **324.** Viscoelastic properties of gamma-irradiated calcium silicate hydrates. **E. Tajuelo Rodriguez**, W. Hunnicutt, P. Mondal, Y. Le Pape

11:45 GEOC **325.** Fundamental mechanisms of heat transport in calcium silicate hydrates. **M. Abdolhosseini Qomi**

Section D

San Francisco Marriott Union Square
Sutter 1-3

Mineral Nucleation: Transient Intermediates & Phase Transitions

S. L. Riechers, *Organizer*

B. Legg, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 GEOC **326.** Is classical nucleation theory valid for ice nucleation? **L. Lupi**, V. Molinero

8:35 GEOC **327.** Withdrawn.

9:05 GEOC **328.** Nucleation in the condensed phase: The role of local solvation in informing an accurate solution model for $CaCO_3$ solutions. **C.J. Mundy**, E. Fetisov, M.D. Baer, G.K. Schenter, J. Siepmann, S. Kathmann

9:25 GEOC **329.** Dynamical nucleation in the condensed phase. **G.K. Schenter**, E. Fetisov, M.D. Baer, S. Kathmann, J. Siepmann, C.J. Mundy

9:45 Intermission.

10:05 GEOC **330.** Heterogeneous nucleation of $CaCO_3$: Thermodynamics and kinetics. **Y. Jun**, Q. Li

10:35 GEOC **331.** Nucleation and epitaxy-mediated phase transformation of a precursor cadmium carbonate phase at the calcite/water interface. **S.L. Riechers**, K. Rosso, S.N. Kerisit

10:55 GEOC **332.** Pseudomorphic growth of cerussite during replacement of calcite micro-crystals. **K. Yuan**, S. Lee, V. De Andrade, N.C. Sturchio, P. Fenter

11:15 GEOC **333.** Relaxation dynamics toward crystallization in amorphous carbonate precursors and the role of water. **A. Koishi**, A. Fernandez-Martinez, B. Ruta, F. Zontone, M. Jimenez-Ruiz

11:35 GEOC **334.** Insight into $CaCO_3$ nucleation from the liquid-liquid phase diagram predicted by COSMO-RS. **M. Andersson**, S. Stipp, K. Dideriksen

Advances in Resource Recovery & Conservation in Water Systems

Sponsored by ENVR, Cosponsored by AGFD, CEI and GEOC

Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOC

THURSDAY AFTERNOON

Section A

San Francisco Marriott Union Square
Union Square North

Environmental Challenges & Solutions in Unconventional Oil & Gas Development

Cosponsored by ENVR

D. Alessi, J. Blotevogel, T. Borch, S. Flynn, *Organizers*, *Presiding*

1:30 GEOC **335.** Hydraulic fracturing, underground injection control, and drinking water interactions. **R.B. Jackson**, M. Kang, D. DiGiulio

2:00 GEOC **336.** Effect of methane leakage on metal mobilization near a shale gas well. **J. Woda**, A. Wendt, S. Hynek, S. Brantley

2:30 GEOC **337.** Sorption behavior of select aryl phosphates onto surficial soils from the Fox Creek area, AB, Canada. **S.P. Funk**, X. Wang, D. Alessi

2:45 GEOC **338.** High resolution LC-MS analysis of microbial lipid biomarkers as evidence of deep shale microbial life. **A. Hanson**, J. Lipp, K. Hinrichs, P. Mouser

3:00 GEOC **339.** Microbiological evaluation of hydraulic fracturing produced water from 17 Bakken Wells across a 6 month time frame. **D. Lipus**, D. Gulliver, K. Bibby, D. Ross, E. Khan, D. Roy, A. Vikram, R. Hammack

3:15 GEOC **340.** Microbial community dynamics in the hydraulic fracturing water cycle of a newly fractured shale gas well in western Canada. **C. Zhong**, J. Li, S. Flynn, C. Nesbo, B. Lanoil, G. Goss, D. Alessi

3:30 Intermission.

3:50 GEOC **341.** Biodegradation of organic additives and hydrocarbons from flowback water of the Denver-Julesburg Basin: A laboratory study of shallow groundwater conditions. **J.D. Rogers**, J. Rosenblum, E.M. Thurman, I. Ferrer, A.R. Bielefeldt, J.N. Ryan

4:10 GEOC **342.** Biodegradation challenges of dissolved organic carbon in hydraulic fracturing flowback and the identification of its recalcitrant fractions. **J. Rosenblum**, K. Linden, K. Sitterley, B. Ruyle, N. Hull

4:25 GEOC **343.** *In situ biodegradation of ethoxylated surfactants by halotolerant bacteria in a hydraulically fractured shale well*. **M. Volker**, G.J. Getzinger, T. Metz, D.L. Plata, M. Borton, M. Wilkins, S. Welch, D. Cole, K. Wrighton, P. Mouser

4:40 GEOC **344.** Emissions of air toxics, ozone precursors, and methane from production sites and new well drilling and completion activities in the Piceance and Denver-Julesburg basins of Colorado. **J.L. Collett**, A. Hecobian, A. Clements, Y. Zhou, K. Shonkwiler, L. MacDonald, N. Hilliard, Y. Desyaterik, B. Wells, D. Weber, J. Pierce, J. Ham

5:00 GEOC **345.** Characteristics, sources, and formation of atmospheric aerosol in the Bakken oil and gas extraction region. **A. Evanoski-Cole**, K.A. Gebhart, B.C. Sive, Y. Zhou, S. Capps, D. Day, A. Prenni, M. Schurman, A. Sullivan, Y. Li, J. Hand, B. Schichtel, J.L. Collett

5:15 GEOC **346.** Capturing methane from the atmosphere. **H. Gokturk**

Section B

San Francisco Marriott Union Square
Union Square South

Contaminants Transport, Uptake & Remediation at Contaminated Sites

Cosponsored by ENVR

B. H. Jeon, Y. Sik Ok, *Organizers*

M. B. Kurade, D. Tsang, *Organizers*, *Presiding*

1:30 GEOC **347.** Mobility and phytoavailability of As and Pb in a contaminated soil using pine sawdust biochar under dynamic redox conditions. **J. Rinklebe**, J. Beiyuan, Y. Awad, F. Felix Beckers, D. Tsang, Y. Sik Ok

2:00 GEOC **348.** Impact of biochar amendment on trace metals speciation in agricultural soils. **D. Alessi**, M. Alam, M. Cossio, B. Bishop, W. Hao, L. Swaren, K. Snihur, T. Warchola, K. von Gunten, S. Flynn, Y. Sik Ok, K. Konhauser

2:30 GEOC **349.** Characterization of colloids in abandoned mine drainage. **M.M. McGuire**, S.L. Bradley, R.A. Bergin, R.M. Wendell, E.K. Herman

2:50 GEOC **350.** Urinary metabolites of polycyclic aromatic hydrocarbons in pregnant women and its association with a biomarker of oxidative stress. **Y. Guo**, P. Wu, L. Shi, E. Zeng

3:10 Intermission.

3:25 GEOC **351.** Utilization of microalgae for the removal of Emerging Contaminants (ECs) from aqueous phase: A bioremedial approach. **M.B. Kurade**, M.M. El-Dalatony, S. Chang, B. Jeon

3:50 GEOC **352.** Distribution of antimony in roadside soils. **C. Foeldi**

4:10 GEOC **353.** Can nitrocellulose possibly control the release of energetic materials from fired munition residues? **D.T. Kuo**, M. Simini, H.E. Allen

4:30 GEOC **354.** Reactive transport of U from co-occurring U(IV) and U(VI) phases in abandoned U mine waste sites. **S. Avasarala**, C. Hirani, A.M. Ali, P. Lichtner, A. Brearley, M. Spilde, E. Peterson, K. Artyushkova, J.M. Cerrato

4:50 GEOC **355.** Engematic behaviour of hexavalent chromium in a superfund site. **J. Fischel**

Section C

San Francisco Marriott Union Square
Savoy

Mineral Nucleation: Transient Intermediates & Phase Transitions

B. Legg, *Organizer*

S. L. Riechers, *Organizer, Presiding*

1:30 GEOC **356.** Accelerated nucleation and polymorph selection with trace additives: Theory and simulation. G. Poon, T. Lemke, C. Peter, V. Molinero, **B. Peters**

2:00 GEOC **357.** Impact of anionic and cationic impurities on the nucleation and growth of nano-Goethite. **S.C. Myneni**, N.M. Crompton, M. Frith, J. Majzlan, S.L. Bernasek

2:30 GEOC **358.** Quantitative analyses of the mechanisms of iron (oxyhydr) oxide nucleation. **J. Scheck**, D. Gebauer

3:00 GEOC **359.** Kinetic study of apoferritin-catalyzed biomineralization of α-MnOOH nanoparticles. **Y. Hui**, H. Jung, Y. Jun

3:30 Intermission.

3:50 GEOC **360.** Withdrawn.

4:10 GEOC **361.** First principles simulation of solid-state transformation of ferrihydrite to goethite. **M. Sassi**, A.M. Chaka, K.M. Rosso

4:30 GEOC **362.** Chemical physics of condensed phase clusters. **S. Kathmann**

4:50 GEOC **363.** Nucleation, growth, and transformation of calcium phosphate minerals in multi-scale nucleation sites of collagen fibrils. **D. Kim**, B. Lee, S. Thomopoulos, Y. Jun

5:10 GEOC **364.** Withdrawn.

Advances in Resource Recovery & Conservation in Water Systems

Sponsored by ENVR, Cosponsored by AGFD, CEI and GEOC

Aquatic Photochemistry

Sponsored by ENVR, Cosponsored by GEOCz

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HIST

Division of the History of Chemistry

S. Rasmussen, *Program Chair*

BUSINESS MEETINGS:
HIST Executive Committee Meeting, 5:00 PM: Sun

SUNDAY MORNING

Section A

Grand Hyatt San Francisco

Warfield

General Papers

S. C. Rasmussen, *Organizer*

J. S. Jeffers, *Presiding*

8:30 HIST **1.** Concentration of power: Alchemy, mercantilism and the *Vitrum Causticum* of Ehrenfried Walter von Tschirnhaus. **N. Zumbulyadis**, A.F. Zumbulyadis

9:00 HIST **2.** Pioneer of pyridine chemistry: Aleksei Yevgen'evich Chichibabin (1871-1945). **D.E. Lewis**

9:30 Intermission.

9:45 HIST **3.** Overview of the discovery of ruthenium. **P. Villarreal**, C. Hahn

10:15 HIST **4.** Richard Willstätter in Munich. **M.O. Senge**

10:45 HIST **5.** History of cuprene: Polymerization of acetylene via electric discharge. **S.C. Rasmussen**

SUNDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Warfield

Golden Age of Industrial Chemistry

Cosponsored by SCC and YCC

J. E. Simpson, *Organizer*

M. Grandbois, *Organizer, Presiding*

1:30 Introductory Remarks.

1:45 HIST **6.** Vladimir Nikolaevich Ipatieff: A sesquicentennial of contributions to the chemistry of high-pressure catalysis. **C.P. Nicholas**

2:15 HIST **7.** J.B.F. Herreshoff and the expansion of the chemicals industry in early 20th century New York. **P. Spellane**

2:45 HIST **8.** Golden age of chemistry: The miracle of instant! Polaroid and the amazing chemistry and innovations of instant photography. **J.C. Giordan**

3:15 Intermission.

3:30 HIST **9.** Evolution of innovation. **S.B. Butts**

4:00 HIST **10.** R&D at Union Carbide Tarrytown Technical Center 1959 - 1990. **K.M. Lewis**

4:30 Concluding Remarks & Networking.

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

Textbooks & the Practice of Science: Before, During & After Gutenberg

Sponsored by CINF, Cosponsored by CHED and HIST‡

MONDAY MORNING

Section A

Grand Hyatt San Francisco

Warfield

Chemistry through the Eyes of Non-Chemists: Evolution of the Public Perception of Chemistry

D. Rabinovich, N. V. Tsarevsky, *Organizers*, *Presiding*

8:25 Introductory Remarks.

8:30 HIST **11.** Public embracement of chemistry: An historical perspective. **H.A. Lawlor**

9:00 HIST **12.** Chemistry's public image: A historical look through the pages of C&EN. **M. Torrice**

9:30 HIST **13.** Eighteenth century textbook of chemistry for women: Compagnoni's La Chimica per le Donne. **G.S. Girolami**, V.V. Mainz

10:00 Intermission.

10:20 HIST **14.** Once upon a Christmas cheery in the lab of Shakhashiri: Public engagement for 47 years and counting. **B.Z. Shakhashiri**

10:50 HIST **15.** Image of chemistry in newspaper and magazine ads. **N.V. Tsarevsky**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Textbooks & the Practice of Science: Before, During & After Gutenberg

Sponsored by CINF, Cosponsored by CHED and HIST‡

MONDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Warfield

Chemistry through the Eyes of Non-Chemists: Evolution of the Public Perception of Chemistry

D. Rabinovich, N. V. Tsarevsky, *Organizers*, *Presiding*

1:30 HIST **16.** Rashomon effect: Chemistry through the eyes of other chemists. **J. Seeman**

2:00 HIST **17.** Viewing chemistry through artists' eyes. **P. Goin**, A. De Bettencourt Dias

2:30 HIST **18.** Guilt by association: Dietary recommendations and missed opportunities. **E. Schoffers**

3:00 Intermission.

3:20 HIST **19.** Changing images of chemistry in the public. **B. Bensaude Vincent**

3:50 HIST **20.** Then and now: Art and the visual image of chemistry. **T.I. Spector**

4:20 HIST **21.** Unlikely popularizer of resonance theory in France. **P. Laszlo**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Textbooks & the Practice of Science: Before, During & After Gutenberg

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MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

S. C. Rasmussen, *Organizer*

8:00 - 10:00

26, 28, 32-34. See subsequent listings.

TUESDAY MORNING

Section A

Grand Hyatt San Francisco

Warfield

Chemistry through the Eyes of Non-Chemists: Evolution of the Public Perception of Chemistry

D. Rabinovich, N. V. Tsarevsky, *Organizers*, *Presiding*

8:30 HIST **22.** My experience as science advisor for Breaking Bad. **D.J. Nelson**

9:00 HIST **23.** Stealing the limelight: Interactions between theatre and chemistry. **K. Shepherd-Barr**

9:30 HIST **24.** From the elements to the atomic fire: An operatic perception of chemistry. **J. Andre**

10:00 Intermission.

10:20 HIST **25.** Science communication: The evolving role of postage stamps. **D. Rabinovich**

10:50 HIST **26.** Periodic table of comic books. **J.P. Selegue**, F.J. Holler

11:20 HIST **27.** Public perceptions of chemistry and the Chemical Heritage Foundation. **R.S. Brashear**

11:50 Concluding Remarks.

TUESDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Warfield

Chemistry & the Design of Physical Objects: Innovation from 1950 to the Present

S. Vasko, *Organizer, Presiding*

1:00 HIST **28.** 100 Years of aluminum pioneers: From chemists to architects (1808-1908). **M. Stacey**

1:30 HIST **29.** Chemical architecture: Experiments in urethane foam environments of the 1960s. **G. Converse**

2:00 HIST **30.** Withdrawn.

2:30 Intermission.

2:45 HIST **31.** Second skin: The science and cultural impact of stretch. **C. Schneider**

3:15 HIST **32.** Ease: Using seam bonding technology to create durable shirts for a girl with autism. **C. Glover**, **E. Riley**, **U. Desai**, G. Jun

3:45 HIST **33.** Trading innovation across chemistry and design: A content analysis of synthetic fiber advertisements. **S. Vasko**

4:15 Panel Discussion.

WEDNESDAY MORNING

Section A

Grand Hyatt San Francisco

Warfield

General Papers

S. C. Rasmussen, *Organizer*

N. Balasubramanian, *Presiding*

8:30 HIST **34.** Was Markovnikov's Rule an inspired guess? ...No! **D.E. Lewis**

9:00 HIST **35.** Paul Dirac: A man at the intersection of science and philosophy. **T.J. Fuhrer**

9:30 HIST **36.** Periodic footprints in history, literature and cinema. **L.R. Ohrstrom**

10:00 Intermission.

10:15 HIST **37.** Drug repurposing: A bibliometric analysis by text-mining PubMed. **N. Baker**, S. Ekins, A.J. Williams, A. Tropsha

10:45 HIST **38.** History of water chemistry monitoring and education on the Yukon River Watershed. **L. DeWilde**

I&EC

Division of Industrial and Engineering Chemistry

E. Rosenberg, *Program Chair*

SUNDAY MORNING

Section A

Grand Hyatt San Francisco

Fillmore A

I&EC International Fellow Symposium: Honoring Professor Kew-Ho Lee

J. Dong, *Organizer*

J. Y. Lin, *Presiding*

8:00 I&EC **1.** 30 Years of membrane research in KRICT. **K. Lee**

8:25 I&EC **2.** Bicontinuous biphasic liquid media for catalysis and separations. **D. Lee**

8:45 Intermission.

9:00 I&EC **3.** High pressure high temperature water gas shift reaction in a zeolite membrane reactor. **A. Arvanitis**, X. Sun, P. Smirniotis, J. Dong

9:20 I&EC **4.** Graphene-based membranes for gas and liquid separation. **H. Park**

9:40 I&EC **5.** Thin film nanocomposite membranes for forward osmosis and pressure retarded osmosis. **H. Choi**

10:00 I&EC **6.** Gas separation properties of metal-organic framework membranes: A comparison with zeolite membranes. **J.Y. Lin**

Nanocellulose Processing & Analysis

Novel Processes

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

SUNDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Fillmore B

Ionic Liquids in Separations & Analysis

C. Hawkins, *Organizer*

M. L. Dietz, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 I&EC **7.** Thiol-yne click chemistry-mediated synthesis of cationic lipids for gene transfection purposes. **J. Gaitor**, L. Paull, S. Michael, S. Isern, A. Mirjafari

1:25 I&EC **8.** Ionic liquids for separations of trivalent lanthanides and minor actinides: Combining performance and radiation stability. **I.A. Shkrob**

1:45 I&EC **9.** Task-Specific Ionic Liquids (TSILs) for metal ion separations: A status report. **M.L. Dietz**, C. Hawkins

2:05 I&EC **10.** Efficient enrichment of 1,3-propanediol from fermentation broths using imidazolium dibutylphosphate ionic liquid based methacrylate polymer membranes. **H. Hawkins**, **L. Boyd**, A. Masoumi, C. Slater, M.J. Savelski, B. Kanjilal, I. Noshadi

2:25 I&EC **11.** Ionic liquids as washing media for biogas upgrading by near isothermal chemical absorption. M. Ahrens, T.J. Schubert, **P. von Czarnecki**, F. Ortloff, M. Roschitz, F. Graf

2:45 I&EC **12.** Cation effects on the post-separation mesoscale structure of an HDEHP-derived ionic liquid for removal of lanthanides from spent nuclear fuel. **C.W. Abney**, C. Do, H. Luo, S. Dai

3:05 Intermission.

3:15 I&EC **13.** Methimazole-based amphiphilic ionic liquid crystals. **S.T. Nestor**, B. Heinrich, L. Douce, A. Mirjafari

3:35 I&EC **14.** Phosphonium ionic liquids in biorefinery applications. **B. Schuur**, X. Li, E. Reyhanitash

3:55 I&EC **15.** Extraction chromatographic separation of metal ions using solid-supported ionic liquids: Progress and prospects. **C.A. Hawkins**, M.L. Dietz

4:15 I&EC **16.** Ionic liquid solvents for recovery and analysis of commodity chemicals. **R.E. Del Sesto**, A.T. Koppisch, D. Warner, J. Melessa, D. Thomas, D. Stapleton, C. Migliori, G. Ifijeh, C. Nwokolo, R. Wolsleger, A. Everett

4:35 I&EC **17.** Tailoring Ionic liquids for f-element separation. J. Dehaudt, N.J. Williams, H. Luo, **S. Dai**

4:55 I&EC **18.** Correlation between ionic liquid ionicity and Pt liquid-liquid extraction performances. **I. Billard**, N. Papaiconomou, P. Husson, J. Andasson, M. Traikia

5:15 Concluding Remarks.

Section B

Grand Hyatt San Francisco

Fillmore A

I&EC Division Fellow Award Symposium: Honoring Professor Klavs Jensen

S. Shankar, *Organizer*

A. K. Chakraborty, *Presiding*

1:00 I&EC **19.** Flow hydrogenations with enhanced stereoselectivity, chemoselectivity, and reactivity. **J. Hawkins**

1:30 I&EC **20.** Mechanistic studies of catalytic organic reactions using reaction progress kinetic analysis. **D.G. Blackmond**

2:00 I&EC **21.** Online sensing of palladium in flowing streams. **C.J. Welch**

2:30 I&EC **22.** How to hit HIV where it hurts. **A.K. Chakraborty**

3:00 I&EC **23.** Designing catalysts for activity and selectivity. **A.T. Bell**

3:30 I&EC **24.** Catalysis for sustainable energy. **J.K. Norskov**

4:00 I&EC **25.** Materials design – The last mile in translation from theory to practice. **S. Shankar**

4:30 I&EC **26.** Automated screening, optimization, and production with multistep flow chemistry. **K.F. Jensen**

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

Nanocellulose Processing & Analysis

Process Parameters

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

MONDAY MORNING

Section A

Grand Hyatt San Francisco

Fillmoare A

2017 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Gregg Beckham

S. C. Chmely, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC **27.** Lignin valorization via biological funnelling. **G. Beckham**

8:50 I&EC **28.** Aromatic monomers via stabilization of reactive intermediates in the acid catalyzed depolymerization of lignin. **K. Barta**

9:20 I&EC **29.** Catalytic processing for the hybrid conversion of lignin into biodiesel. **M. Foston**

9:50 Intermission.

10:10 I&EC **30.** Stabilization with formaldehyde facilitates the high-yield production of monomers from lignin during integrated biomass depolymerization. **J.S. Luterbacher**

10:40 I&EC **31.** Toward a fundamental understanding of carbonyl hydrogenation in condensed media. **J. Bond**, O.A. Abdelrahman

11:10 I&EC **32.** Role of lignin in the performance of regenerating lignocellulosic materials. **N. Labbé**, J. Wang, R. Boy, J.K. Keum, D.A. Cullen, J. Chen, D. Harper, L. Tetard, T.G. Rials, A.K. Naskar

11:40 Concluding Remarks.

Section B

Grand Hyatt San Francisco

Fillmore B

Symposium in honor of Michelle Cummings, ACT Fellow

Financially supported by Dow Corning Corporation

J. McDonald, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 I&EC **33.** Fluorosilicone polymers and fluorosilicone diblock copolymers. **S. Clarson**

8:40 I&EC **34.** Fracture and thermal aging of resin-filled silicone elastomers. **K.R. Shull**

9:10 I&EC **35.** Tailored silicone structures lead to tailored silicone properties. **M.A. Brook**, J. Morgan, A. Schneider, S. Laengert

9:40 Intermission.

9:55 I&EC **36.** Silsesquioxane copolymers for lighting. **S. Swier**

10:25 I&EC **37.** Effects of time and temperature on mechanical properties of silicone hot-melt adhesives. **G.V. Gordon**, L. Yan, D.A. Dillard

10:55 I&EC **38.** Role of thermal stability in siloxane applications. **M.R. Cummings**

11:25 Concluding Remarks.

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

Nanocellulose Processing & Analysis

Properties

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

MONDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Filmore A

2017 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Jinlong Gong

D. Flaherty, *Organizer, Presiding*

R. M. Rioux, *Presiding*

1:30 I&EC **39.** Synthesis and processing of copper-based nanowires for use as transparent conductors. **B.J. Wiley**

2:00 I&EC **40.** Collapsed polymer-directed synthesis of inorganic nanostructures with complex geometries. Z. Huang, Y. Liu, J. Gong, **Z. Nie**

2:30 I&EC **41.** Preferential binding of Polyvinylpyrrolidone (PVP) is not responsible for shape control in Ag nanoparticle synthesis. Z. Chen, J. Chang, C. Bala, **R.M. Rioux**

3:00 I&EC **42.** Dumpsites as 21st century mines: Affordable recovery of rare-earths and critical materials from e-waste. C. Frankiewicz, B. Chang, **M. Thuo**

3:30 I&EC **43.** Production of chemicals from ethanol: Unexpected selectivity within aldol addition reaction networks. T. Moteki, A. Rowley, H. Zhang, **D. Flaherty**

4:00 I&EC **44.** C-H bond activation in glucose oxidation over CuO. **Y. Yang**

4:30 I&EC **45.** Effective charge carrier utilization in photocatalytic conversions. **J. Gong**

5:15 Award Presentation and Remarks.

Section B

Grand Hyatt San Francisco

Fillmore B

ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

J. Frommer, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 I&EC **46. Award Address** (ACS Award in Industrial Chemistry sponsored by the ACS Division of Industrial & Engineering Chemistry). Evolution of AFM in chemical analysis. **J. Frommer**

1:50 I&EC **47.** Atomic force microscopy: Past, present, and future. **M. Tortonese**

2:20 I&EC **48.** Spectroscopy on the nanoscale with photo-induced force microscopy. **T.R. Albrecht**

2:50 I&EC **49.** Advances in APM-mediated 3D nanoprinting. **G. Liu**

3:20 I&EC **50.** Heatable scanning probes, from data storage to nanolithography. **A. Knoll**

3:50 I&EC **51.** Manipulative force microscopy: Pulling molecular chains and nanoribbons. **E. Meyer**

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

4:20 I&EC **52.** Quantitative and qualitative nanomechanical measurements with AFM: Recent advances and thoughts for future directions. **D. Yablon**

4:50 I&EC **53.** Advances in AFM-based IR spectroscopy and mass spectrometry for high-resolution chemical characterization. **E. Dillon**

5:20 I&EC **54.** Advances in ambient and liquid AFM: Nanoscale structure and dynamics. **R. Proksch**

5:50 Concluding Remarks.

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

Nanocellulose Processing & Analysis

Fundamentals

Sponsored by CELL, Cosponsored by AGFD, ANYL, CHAS and I&EC

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Mechanistic Studies of Catalysis in Photocatalytic & Photoelectrodes

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

E. Rosenberg, *Organizer*

8:00 - 10:00

10, 28, 37. See previous listings.

96, 98, 103, 107, 116, 118, 121, 123, 125-126, 134, 136. See subsequent listings.

TUESDAY MORNING

Section A

Grand Hyatt San Francisco
Filmore A

2016 E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in honor of Michael M. Thackeray

Y. Shao-Horn, *Organizer, Presiding*

E. S. Takeuchi, *Presiding*

8:00 Introductory Remarks.

8:05 I&EC **55.** Evolution of lithium-ion batteries: Personal reflections. **M. Thackeray**

8:35 I&EC **56.** Development of manganese-rich, high-capacity lithium-ion cells. **J. Croy**

8:55 I&EC **57.** Synthesis and analysis of NCM cathode materials for high performance Li-Ion batteries. **M.A. Fetcenko**

9:25 I&EC **58.** Renaissance of $LiMn_2O_4$ spinel. **C.S. Johnson**

9:45 I&EC **59.** Gassing reactions of NCM cathodes operated at high voltage. **H. Gasteiger**

10:15 I&EC **60.** Safe, high-voltage rechargeable batteries. **J.B. Goodenough**

10:45 I&EC **61.** High energy density rechargable batteries: A little history and a look into the future. **M. Whittingham**

11:15 I&EC **62.** Investigating the complex chemistry of functional energy storage systems: The need for a multiscale (molecular- to meso-scale) perspective. **E.S. Takeuchi**, K.J. Takeuchi, A.C. Marschilok

11:35 I&EC **63.** Simplify your experiments: Simple three electrode and full cell measurements for better understanding of lithium ion battery materials. **M. Winter**

12:05 I&EC **64.** In operando neutron diffraction studies of battery materials. **K. Edstrom**

Section B

Grand Hyatt San Francisco
Fillmore B

2017 ACS Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Helen Sneddon

S. G. Koenig, *Organizer, Presiding*

J. C. Colberg, *Presiding*

8:00 Introductory Remarks.

8:05 I&EC **65.** Nickel-catalyzed asymmetric transfer hydrogenation of unsaturated bonds. **J. Zhou**

8:30 I&EC **66.** Passing on the medicinal chemistry baton: University of Nottingham and GlaxoSmithKline collaborative research projects. **T. McInally**

8:55 I&EC **67.** Supporting the transition to increased sustainability in common reactions. **A.J. Watson**

9:20 Intermission.

9:25 I&EC **68.** Sustainable chemistry in pharmaceutical R&D: Successes, works in progress, and future challenges. **H. Sneddon**

10:00 I&EC **69.** Synthesis of cyclic compounds by organocatalytic/multicomponent reactions sequence and photochemical approaches. **M. Paixao**

10:25 I&EC **70.** Development of sustainable processes for pharmaceutical R&D. **K. Wheelhouse**

10:50 Intermission.

10:55 I&EC **71.** Making medicines more sustainably: Efforts of the ACS Green Chemistry Institute Pharma Roundtable (GCIPR). **S.G. Koenig**

11:15 I&EC **72.** Green chemistry at Pfizer – Applications to the oncology portfolio. **P. Richardson**

11:35 I&EC **73. Award Address** (ACS Award for Affordable Green Chemistry sponsored by Dow Chemical Company & endowed by Rohm & Haas Company). Green synthesis of Viagra as a springboard for promoting green chemistry in the pharmaceutical industry. **P. Dunn**

11:55 Concluding Remarks.

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Molecular & Bio-Inspired Photocatalysts

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Sponsored by CATL, Cosponsored by ENVR and I&EC

TUESDAY AFTERNOON

Section A

Grand Hyatt San Francisco
Filmore A

2016 E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in honor of Michael M. Thackeray

Y. Shao-Horn, *Organizer*

Y. Lu, D. R. Rolison, *Presiding*

1:30 I&EC **74.** Insights into lithium battery cathodes from powder diffraction data. **B. David**

2:00 I&EC **75.** Tale of spinels: From Li-Ion to Mg battery electrodes. **J. Cabana**

2:30 I&EC **76.** Simulated synthesis, characterisation and performance of binary and ternary metal oxide electrodes. **P. Ngoepe**

3:00 I&EC **77.** Revealing the conversion mechanism of Co_3O_4 during lithiation from first principles calculations. **C. Wolverton**

3:30 I&EC **78.** Spinels and layered manganates: New NMR approaches to characterize order and disorder. **C.P. Grey**

4:00 I&EC **79.** Key challenges in the development of solid state lithium batteries. **J. Janek**

4:30 I&EC **80.** Something from nothing: Enhancing cathode electrochemical charge storage with cation vacancies. **D.R. Rolison**, J.W. Long

4:50 I&EC **81.** Activating Oxygen Redox for Energy Storage. **Y. Shao-Horn**

5:10 Concluding Remarks.

Recent Developments in TSCA Regulation: New Requirements for Chemicals in Commerce

Sponsored by CHAL, Cosponsored by CHAS, ENVR and I&EC

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Novel Photocatalytic & Photoelectrode Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Sponsored by CATL, Cosponsored by ENVR and I&EC

WEDNESDAY MORNING

Section A

Grand Hyatt San Francisco
Filmore A

I&EC Division Early Career Fellow Symposium: Honoring Dr. Leigh Martin

G. A. Fugate, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 I&EC **82.** Probing the solution chemistry of f-element interactions with hydroxycarboxylic acids. **K.L. Nash**

8:25 I&EC **83.** Recent advances in development of the sodium bismuthate process for the oxidation and separation of Am from used nuclear fuel. **J. Law**, B. Mincher, R. Tillotson, N. Schmitt

8:45 I&EC **84.** Determining DTPA complexation kinetics. **K. Larsson**, S.P. Mezyk

9:05 I&EC **85.** Gamma radiolysis of americium-nitric acid solutions. **G.P. Horne**, S.P. Mezyk, B. Mincher, T.S. Grimes

9:25 Intermission.

9:45 I&EC **86.** Role of organic radical cation chemistry in separation ligand degradation. **S.P. Mezyk**, B. Mincher, P.R. Zalupski

10:05 I&EC **87.** Savannah River site's quest to recover plutonium-244 from the mark-18A targets. **N. Bridges**

10:25 I&EC **88.** Separation of minor actinides from lanthanides in acidic media using symmetric and asymmetric dithiophosphinic acid extractants. **D.R. Peterman**

10:45 Concluding Remarks.

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Spectroscopy & Microscopy of Photocatalytic & PEC Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Fundamental Structure-Activity Relationships: The Interface of Operando with Physical Sciences

Sponsored by CATL, Cosponsored by ENVR and I&EC

2017 E.V. Murphree Award in Industrial & Engineering Chemistry: Symposium in honor of Eleftherios T. Papoutsakis

Sponsored by BIOT, Cosponsored by I&EC

WEDNESDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Filmore A

I&EC Division Early Career Fellow Symposium: Honoring Dr. Leigh Martin

G. A. Fugate, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 I&EC **89.** Exploiting properties of alkali titanates for separations and biomedical applications. **D.T. Hobbs**, K.M. Taylor-Pashow, J.L. Drury, J.C. Wataha

2:25 I&EC **90.** Modified DTPA ligand systems for simplified trivalent actinide-lanthanide separations based on the TALSPEAK process. J. Jones, M.H. Langford, A. Geist, P. Panak, P. Kaden, C. Adam, N. Adam, C.A. Sharrad, L. Martin, **L.S. Natrajan**

2:45 I&EC **91.** Separations in advanced nuclear fuel cycles. **C.A. Sharrad**, A.C. Edwards, H. Lambert, Z. Bikbajeva, R. Foster, T. Kerry, R.C. Whitehead, L.M. Harwood

3:05 I&EC **92.** Real-time direct measurement of extraction kinetics and speciation in solvent extraction systems. **M.P. Jensen**, R.G. McDowell, L. Martin

3:25 Intermission.

3:45 I&EC **93.** Pertechnetate extraction from aqueous environments. **P.D. Benny**, S.C. Bottorff, L. Martin

4:05 I&EC **94.** Study of 4f series metal binding kinetic phenomena by a TALSPEAK extractant via UV-Vis spectrophotometry in a mixed liquid-liquid separation system. **R.G. McDowell**, S.P. Mezyk, L.R. Martin

4:25 I&EC **95.** Wear and tear: Degradation effects in f-element separation science. **L. Martin**

4:45 Concluding Remarks.

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Devices, Assemblies & Hybrid Processes

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Fundamental Structure-Activity Relationships: The Interface of Operando with Physical Sciences

Sponsored by CATL, Cosponsored by ENVR and I&EC

WEDNESDAY EVENING

Section A

Moscone Center

Hall D

General Posters

E. Rosenberg, *Organizer*

6:00 - 8:00

I&EC **96.** Anatase pigment production by hydrolysis of unenriched $TiOSO_4$ solution via short sulfate process. **C. Tian**

I&EC **97.** Metal-organic framework materials in microfluidics: Synthesis and functional integration. K. He, **Z. Li**, K. Yeung

I&EC **98.** High throughput water disinfection using pulsed electric field. H. Leung, **Q. Chang**, K. Yeung

I&EC **99.** Porous carbons prepared by soft-template method as electrodes for supercapacitor. **S. Park**, J. Lee

I&EC **100.** Carbon capture using ammonia activated carbons from polysaccharides. **S. Park**, J. Lee

I&EC **101.** Catalytic preparation of ammonium carbonate using urea as a raw material. **S. Park**, J. Lee

I&EC **102.** Alkylation of benzene with ethylene in the presence of zeolite catalyst: Mathematical modelling of reactor. **E. Khlebnikova**, E. Ivashkina, I. Dolganova, I. Dolganov, S. Koshkin, E. Yurev

I&EC **103.** Sensing and removal of Hg^{2+} from contaminated water, and beneficiation of the gettered material in organic reduction reaction and hydrogen production. **A. Malek**, T. Thomas, P. Edamana

I&EC **104.** Carbon-modified nanofiltration membrane-based advanced oxidation reactor for endocrine disrupting compound removal. Y. Li, **W. Han**, K. Yeung

I&EC **105.** Novel approaches to the chemical application of electro chemicals for conducting materials. E.J. Parish, G. Ren, **H. Honda**, **M. Hsiao**, T. Wei

I&EC **106.** Novel approaches to the chemical synthesis and characterization of D-sigma-A molecules for molecular rectification. E.J. Parish, G. Ren, Y. Lo, **H. Honda**, **H. Shyu**, T. Wei

I&EC **107.** Bactericidal activity and biosafety studies of high-intensity narrow-wavelength (Hi-NW) light. **Q. Chang**, N. Zhan, N. Wong, J. Kwan, K. Yeung

I&EC **108.** Self-assembled ionic liquid crystals and their ion transport behavior. **S. Park**, J. Lee

I&EC **109.** Investigating the stability of tris(acetylacetonato)vanadium(III) complex. **J. Lee**, J. Lee

I&EC **110.** Properties of metal complexes as the active materials for the redox flow batteries. **J. Lee**, J. Lee

I&EC **111.** Fate of triazole fungicides in softwood after environmental exposure. **K. Kukowski**, C.A. Sedgeman, V. Martinská, E.I. Kozliak, S. Fisher, A. Kubatova

I&EC **112.** Supported bicyclic amidine ionic liquids as a potential CO_2/N_2 separation medium. **J.A. Schott**, C. Do-Thanh, S.M. Mahurin, D. Jiang, S. Dai

I&EC **113.** Withdrawn.

I&EC **114.** Novel approaches to the chemical synthesis and characterization of alkyl phenols derivatives with various side chains. G. Ren, E.J. Parish, **H. Honda**, **M. Hsiao**, T. Wei

I&EC **115.** Gels as precursors in the preparation of catalysts and their films. **D.L. Perry**, C. Perrino

I&EC **116.** Metal ions in inks studied by synchrotron x-ray fluorescence microprobe techniques. **D.L. Perry**, T. Wilkinson

THURSDAY MORNING

Section A

Grand Hyatt San Francisco

Conference Theatre

General Papers

E. Rosenberg, *Organizer*

F. K. Wood-Black, *Presiding*

8:00 Introductory Remarks.

8:05 I&EC **117.** Synthesis and evaluation of a series of ionic liquids functionalized with dipicolinate complexants. **A.J. Ferry**, C. Hawkins

8:25 I&EC **118.** Withdrawn.

8:45 I&EC **119.** Indirect Ocean Capture: Applications and analysis of membranes for CO_2 capture. **C.P. de Lannoy**, J. Rivest, M. Eisemann, S. Karnitz, A. Jose, R. DeVaul, K. Cooper

9:05 I&EC **120.** Study on combined cooling and antisolvent crystallization of L- asparagine monohydrate. **M. Lenka**, D. Sarkar

9:25 I&EC **121.** Design and operation experience of hexagon structured cyclone separator using mathematical models and computational fluid dynamic methodology. **T. Zhang**, C. Liu, K. Guo

9:45 I&EC **122.** Porous carbons derived from biomass and their application for the carbon capture. **S. Park**, J. Lee

10:05 Intermission.

10:15 I&EC **123.** Non-uniform gas solids distribution and its effects on performance of fluidized bed reactors. **C. Zhang**, W. Qian, F. Wei

10:35 I&EC **124.** Prediction of the vapor-liquid equilibrium of chemical reactive systems containing formaldehyde using the COSMO-RS method. **Z. Bai**, **H. Liu**, Y. Liu, L. Wu

10:55 I&EC **125.** Understanding the activity of Na_2WO_4/Mn/SiO_2 catalyst for the oxidative coupling of methane based on the optimization of reaction parameters. **S. Yoon**, J. Choi, D. Suh, J. Ha, M. Park, K. Song

11:15 I&EC **126.** Selective ethylene oxidation to EDC in Chemetry's Shuttle™ process. **M.K. Leclerc**, T.A. Albrecht, E.A. Cole

11:35 I&EC **127.** Dry pressure drop within Winpak-mechanism and optimization. **W. Qi**, K. Guo, C. Liu

11:55 I&EC **128.** Transformation behavior of MoO_3 as oxygen carrier for chemical looping gasification of coal and its reaction mechanism. G. Wu, **W. Li**, T. Wiltowski

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Engineering Operando to Larger Scale: Shaped Catalysts & Process Control

Sponsored by CATL, Cosponsored by ENVR and I&EC

THURSDAY AFTERNOON

Section A

Grand Hyatt San Francisco

Conference Theatre

General Papers

E. Rosenberg, *Organizer*

F. K. Wood-Black, *Presiding*

1:30 Introductory Remarks.

1:35 I&EC **129.** Synthesis of 9-fluorenylmethanol and the coproduction of phenanthrene from crude anthracene. H. Mu, **W. Li**, C. Ye

1:55 I&EC **130.** Chaotropic agents for amidoxime adsorbent pretreatments. **R.T. Mayes**

2:15 I&EC **131.** Modeling and optimization of ultrasound assisted crystallization of L asparagine monohydrate. **S. Bhoi**, D. Sarkar

2:35 I&EC **132.** Chromatographic purification of 5,6 cis-dihydroxycyclohexane 1,3-diene, the precursor to poly(para-phenylene). **B. Ikizer**, A. Polanco, N. Orbey, C. Lawton

2:55 I&EC **133.** Reaction kinetics of formaldehyde–water–1,3,5-trioxane–sulfuric acid system at 371.15 K. **X. Zhang**, Y. Hu

3:15 Intermission.

3:25 I&EC **134.** Composite nano-particle synthesis for enhanced photo-catalytic activity of textiles. **G. Basim**, A. Cerhan

3:45 I&EC **135.** Experimental investigation of the effects of the geometry on liquid radial and axial distribution in modular catalytic structured packing. C. Liu, **W. Xiang**

4:05 I&EC **136.** Electroplating of active metals from aqueous systems for accessing materials of the future. **H.B. Nulwala**, X. Zhou, J. Watkins

4:25 I&EC **137.** Withdrawn.

Operando Methodology at the Junction between Fundamental Chemistry & Chemical Engineering

Engineering Operando to Larger Scale: Shaped Catalysts & Process Control

Sponsored by CATL, Cosponsored by ENVR and I&EC

‡ *Cooperative Cosponsorship*

INOR

Division of Inorganic Chemistry

S. Koch and N. Radu, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark (see *NUCL*, Sun, Mon, Tue)

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten (see *NUCL*, Tue)

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory (see *PHYS*, Sun, Mon, Tue, Wed)

Metalloprotein-Initiated Signaling Transduction Response to Redox Stress (see *BIOL*, Tue)

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium (see *PROF*, Sun, Mon)

Support & Activator Effects on Metal Mediated Polymerization (see *PMSE*, Mon, Tue)

SUNDAY MORNING

Section A

Moscone Center
2009

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Nilay Hazari

W. H. Bernskoetter, A. Valentine, *Organizers*

J. E. Bercaw, *Presiding*

9:00 INOR **1.** Towards a thermochemical hydrogen-affinity scale for oxide materials, and its implications in reactivity and catalysis. **J.M. Mayer**, J. Peper, J. Lora, S. Laga, D. Damatov, C. Valdez, J. Peng, B. Broudy

9:25 INOR **2.** Bonding in pentalene complexes and their recent applications. **J.C. Green**

9:50 INOR **3.** Small molecule activation with molybdenum complexes supported by diphosphine-arene ligands. **T. Agapie**

10:15 Intermission.

10:25 INOR **4.** Reversible C-H bond cleavage in the formation of cationic iridium alkoxycarbenes from ethers. **N.D. Schley**

10:50 INOR **5.** Siderophore-Promoted release of titanium(IV) from metal oxide materials. **A. Valentine**

11:15 INOR **6.** Electronic structures of diplatinum complexes. **H.B. Gray**

11:40 INOR **7.** Near-miss synthesis of a noble gas compound in 1933: Could it have been Harry Gray award-worthy? **J.A. Labinger**

Section B

Moscone Center
2011

Celebrating 60 Years of the Division of Inorganic Chemistry

The Early Days of the Division of Inorganic Chemistry (DIC)

M. J. Clarke, *Organizer*

D. C. Crans, *Organizer, Presiding*

T. J. Marks, A. P. Sattelberger, *Presiding*

8:30 Introductory Remarks.

8:40 INOR **8.** Sixty years of inorganic chemistry. **H.B. Gray**

9:10 INOR **9.** Synthesis and properties of selected transition metal complexes over half a century - a retrospective. **S.J. Lippard**

9:40 INOR **10.** My experiences inside the Division of Inorganic Chemistry. **D.J. Nelson**

10:10 Intermission.

10:25 INOR **11.** Inorganic and supramolecular pincer chemistry. **K. Bowman-James**

10:55 INOR **12.** Whither goest inorganic chemistry: What goes around, comes around. **R. Eisenberg**

11:25 INOR **13.** How the Division of Inorganic Chemistry brought the ACS into the 21st Century: E-Lections and the DIC's first ChemLuminary Award. **M.J. Clarke**

Section C

Moscone Center
2016

Undergraduate Research at the Frontiers of Inorganic Chemistry

Coordination Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

B. B. Sears, *Presiding*

9:00 Introductory Remarks.

9:05 INOR **14.** Selective f-element extraction utilizing tripodal CMPO ligands. **E.J. Werner**, S.M. Biros, M. Patterson, A.K. Mulville, E.K. Connor

9:25 INOR **15.** N-heterocyclic thione and selones: New tricks for old dogs. **D. Rabinovich**

9:45 INOR **16.** Exploring the reactivity of hexaphenylcarbodiphosphorane with electron-deficient metallic species. **G. Risica**, C.D. Abernethy, M. Findlater

10:05 INOR **17.** Structure and properties of coordination polymers containing conformationally flexible dipyridylamide ligands: An introductory undergraduate research program at Lyman Briggs College at Michigan State University. **R.L. Laduca**, T.A. Beard, J.Z. Travis

10:25 Intermission.

10:40 INOR **18.** Ligand replacement on 1D and 2D coordination polymers. **B.J. Johnson**, M. Johnson, N. Beattie

11:00 INOR **19.** Synthesis, electronic structure, and reactivity of iron complexes bearing donor-modified BIAN ligands. **H.M. Hoyt**, G.N. Tran, C.C. Cody, M. Takemura, L. Darko, A. Volkov, E.Y. Martinez, W.R. Fuller, J.M. Darmon, C.E. Schulz, K.A. Wheeler

11:20 INOR **20.** Synthesis and characterization of cobalt(II) SNS pincer model complexes for liver alcohol dehydrogenase. **J.R. Miecznikowski**, **S. Bonitatibus**, J. Jasinski, L. Li

11:40 INOR **21.** Peptoid ligands: Bioinspired chelators for lanthanide and actinide complexation. **A. Ricano**, I. Captain, G. Deblonde, R.J. Abergel

Section D

Moscone Center
2018

ACS Award in Inorganic Chemistry: Symposium in honor of Lawrence Que, Jr.

M. J. Maroney, E. L. Que, *Organizers*

T. A. Jackson, J. Kovacs, *Presiding*

8:30 Introductory Remarks.

8:35 INOR **22.** Diiron enzymes in antibiotic biosynthesis: Similar metal centers - different chemistry. A.J. Komor, C.J. Knoot, A. Jasniewski, B.S. Rivard, L. Que, **J.D. Lipscomb**

9:00 INOR **23.** Mössbauer, EPR and DFT studies of Fe(V)=O, Fe(IV) Fe(IV) and Fe(III) Fe(IV) complexes of biological relevance. **E. Munck**

9:25 INOR **24.** Metal selectivity in nickel trafficking proteins. **M.J. Maroney**, C.E. Carr, H.Q. Hu, H. Huang, R.C. Johnson, S.L. Ciurli, D.S. Merrell

9:50 INOR **25.** DNA repair glycosylase MUTYH: From Fe-S clusters to MAP. **S.S. David**

10:15 Intermission.

10:30 INOR **26.** Mechanistic enzymology of tryptophan oxidizing enzymes. **A. Liu**

10:55 INOR **27.** Gallium complexes targeting FepA: An inorganic approach to fighting antimicrobial resistance. **V.C. Pierre**

11:20 INOR **28.** Metal scaffolds for biological sensing using ^{19}F magnetic resonance imaging. **E.L. Que**

11:40 INOR **29.** Spectroscopic and kinetic studies of a bifunctional α-ketoglutarate dependent non-heme iron enzyme, AsqJ. **Y. Guo**, J. Li, J. Lee, J. Dicks, R. Fan, W. Chang

12:00 INOR **30.** Developing x-ray spectroscopic toolkits for mechanistic studies of cobalt and nickel catalysts. **F. Li**

Section E

Moscone Center
2020

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

E. J. McLaurin, *Organizer*

K. R. Kittilstved, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR **31.** Mechanistic investigations of colloidal metal chalcogenide nucleation and growth. **J.S. Owen**, M.P. Campos, I. Rreza

9:05 INOR **32.** Germanium alloy nanocrystals and hollow spheres prepared via colloidal synthesis. **S. Kauzlarich**, K. Tabatabaei, K.A. Newton, X. Qi

9:35 INOR **33.** Inorganic-Capped luminescent InP nanocrystals. **E.J. McLaurin**

10:05 Intermission.

10:20 INOR **34.** High throughput nanomaterial synthesis and its application to technology. **G.F. Strouse**

10:50 INOR **35.** Design of multi-functional nanocrystal membranes and the fabrication of thin film nanocrystal devices. **C.B. Murray**, Y. Wu, N. Gogotsi, T. Zhao, N.J. Greybush, D. Straus, D. Jishkariani, K.C. Elbert, C.R. Kagan

11:20 INOR **36.** Dislocation-Driven growth of 1D, 2D and 3D nanomaterials and the applications in lead halide perovskite nanostructures. **S. Jin**, Y. Fu

11:50 INOR **37.** Synthesis of magnetic semiconductor nanostructures. **S.L. Stoll**

Section F

Moscone Center
2022

Sustainability in Electrocatalytic Fuel & Chemical Production

Cosponsored by CATL

L. A. Berben, J. L. Dempsey, *Organizers*

V. Thoi, *Presiding*

8:30 Introductory Remarks.

8:35 INOR **38.** Why is Ni(cyclam)$^{2+}$ a better CO_2 reduction catalyst when supported on a mercury surface? B. Rudshteyn, Y. Wu, J. Froehlich, A. Zhanaidarova, W. Ding, V.S. Batista, **C.P. Kubiak**

9:00 INOR **39.** Engineered biomolecular electrocatalysts for hydrogen evolution from water. **K. Bren**, Y. Guo, B. Kandemir, V. Fourmond

9:25 INOR **40.** Paired electrochemical reactions: A lesson learned from microelectrode arrays and the on-site generation of chemical reagents. **K.D. Moeller**

9:50 INOR **41.** Promoting selective electrocatalytic carbon dioxide reduction through modification of a metal's secondary and outer coordination spheres. **C.C. McCrory**

10:15 INOR **42.** Towards electrocatalytic reduction of carbon dioxide to methanol: Adventures in hydricity. **E.S. Wiedner**, S.A. Burgess, M.J. Wilding, D.L. Miller, M. Helm, J.C. Linehan, A.M. Appel

10:40 Intermission.

10:55 INOR **43.** Mechanistic details of CO_2 reduction processes revealed by pulse radiolysis with time-resolved infrared detection. **D.C. Grills**, K.T. Ngo, J.J. Rochford

11:20 INOR **44.** Rational design of catalysts for fuel generation: Controlling the secondary coordination sphere. D.J. Harrison, E. Jarvis, Z.R. Relethford, **C.A. Caputo**

11:40 INOR **45.** Mechanistic insight into the cleavage and coupling of CO with molybdenum complexes: Toward upgrading oxygenated C_1 precursors. **T. Agapie**

12:05 INOR **46.** H_2 Evolution by metal chalcogenide coordination polymers, highly active molecular models of [NiFe] hydrogenases. **S.C. Marinescu**

Section G

Moscone Center

2024

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

X. Bu, Q. Zhang, D. Zhao, *Organizers*

P. Yang, N. Zheng, *Organizers*, *Presiding*

8:30 INOR **47.** Pingyun Feng - the quintessence of synthetic materials chemistry. **G.D. Stucky**

9:00 INOR **48.** Nanostructured and single phase thermoelectrics. **M.G. Kanatzidis**

9:20 INOR **49.** Interfacial assembly and engineering of ordered functional mesoporous materials. **D. Zhao**

9:40 INOR **50.** Sol-gel assembly of metal chalcogenide nanoparticles into multicomponent architectures. J. Davis, **S. Brock**

10:00 Intermission.

10:30 INOR **51.** Nanostructured and nanoporous materials for energy application. **S.H. Tolbert**

10:50 INOR **52.** Synthesis and applications of conducting polymer nanofibers. **R.B. Kaner**, W.H. Mak, C. Lin, R. Li, D. Maung, X.W. Huang, K. Wang, Y. Wang, T. Farrell

11:10 INOR **53.** Design and synthesis of novel porous materials for energy and environmental applications. **T.M. Nenoff**

11:30 INOR **54.** Synthesis and substitution chemistry of complex bismuth sulfide iodides in sulfur/iodine melts. R.A. Groom, **S.E. Latturner**

11:50 INOR **55.** Spark plasma sintering of Zintl phases. **S. Kauzlarich**, E.L. Kunz Wille, J. Cooley, D. Barrett, N. Grewal

Section H

Moscone Center

3000

Bioinorganic Chemistry

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

M. Knapp, F. Li, *Presiding*

8:00 INOR **56.** Theoretical studies of the mechanism of the second half-reaction step of nitric oxide synthase: Nondynamical electron correlation drives the reaction to the intended products. **I. Shamovsky**, G. Belfield, R. Lewis, F. Narjes, L. Ripa, C. Tyrchan, L. Öberg, P. Sjo

8:20 INOR **57.** Proton-facilitated transformations of molybdenum-oxo compounds as synthetic models for molybdoenzymes. **F. Li**

8:40 INOR **58.** Metal capture and sensing in porous polymers for disease and environmental diagnostics. **S. Lee**, G. Barin, J.R. Long, C.J. Chang

9:00 INOR **59.** Mechanistic investigations of guest binding in a self-assembled Ga_4L_4 host reveals the first example of a conformational selection mechanism in a synthetic host. **C.M. Hong**, D.M. Kaphan, D. Toste, K.N. Raymond, R.G. Bergman

9:20 INOR **60.** Engineering the alpha-ketoglutarate oxygenase FIH for alternate rebound chemistry. **M. Knapp**

9:40 INOR **61.** Urease inhibitors: In search for a key to control a nickel-enzyme. **S.L. Ciurli**

10:00 Intermission.

10:10 INOR **62.** Iron-assisted CO_2 activation at a nickel center. **C. Yoo**, Y. Lee

10:30 INOR **63.** Mechanistic, structural and computational studies of the catalytic multifunctional hemoglobin dehaloperoxidase from *Amphitrite ornata*. **R.A. Ghiladi**, L.M. Carey, N.L. McCombs

10:50 INOR **64.** Mechanistic nuances of hydrogen atom abstraction by the copper(III)-hydroxide unit. **D. Dhar**, G.M. Yee, J.M. Mayer, C.J. Cramer, W.B. Tolman

11:10 INOR **65.** Structure-function studies of tetranuclear iron clusters with a variable interstitial μ_4-atom as models of biological active sites. **C. Reed**, T. Agapie

11:30 INOR **66.** Bio-inspired nonheme iron catalyst: Electrophilic versus nucleophilic iron-based active oxidant – effect on alkane hydroxylation. **S. Kal**, L. Que

11:50 INOR **67.** Withdrawn.

Section I

Moscone Center

3010

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

X. Chen, M. V. Sheridan, *Presiding*

8:30 INOR **68.** Polydiacetylene-(phen) $Ru(bpy)_2$ for cofactor regeneration and CO_2 reduction as an artificial photocatalytic system. **J. Kim**, S. Kim, T. Anjong, H. Lee

8:50 INOR **69.** Bismuth-based double perovskites for non-toxic photovoltaics. **A. Slavney**, T. Hu, A. Lindenberg, H. Karunadasa

9:10 INOR **70.** Three-dimensional graphene nanoribbon-based materials and its applications. **T. Yi**

9:30 INOR **71.** Pulsed-laser synthesis of advanced nanomaterials for water-oxidation catalysis and sunlight capture. **A.M. Mueller**, J.R. Winkler, H.B. Gray

9:50 INOR **72.** Metal chalcogenide coordination polymers as catalysts for the hydrogen evolution reaction. **C.A. Downes**, S. Marinescu

10:10 Intermission.

10:25 INOR **73.** All-in-one, derivatized tandem p^+n-$Si/SnO_2@TiO_2$ water splitting device. **M.V. Sheridan**, T.J. Meyer

10:45 INOR **74.** General strategy for electrocatalytic hydrogen production integrated with oxidative organic upgrading. **Y. Sun**

11:05 INOR **75.** Chemically tailoring two-dimensional transition metal dichalcogenides. **X. Chen**, A.R. McDonald

11:25 INOR **76.** Polydopamine coatings for stabilizing the interface between cobalt-based water oxidation catalysts and electrode. **I. Kim**, Y. Nam

Section J

Moscone Center

3012

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

P. Yin, *Presiding*

8:30 INOR **77.** Electron hopping through double-exchange coupling in a mixed-valence diiminobenzoquinone-bridged Fe_2 complex. **A. Gaudette**, I. Jeon, J.S. Anderson, G.J. Long, F. Grandjean, D. Harris

8:50 INOR **78.** Enhancement of magnetic anisotropy in a heterobimetallic Mn-Bi complex. **T. Pearson**, M. Fataftah, D.E. Freedman

9:10 INOR **79.** Redox series of gallium complexes: Characterization of four oxidation states and electrocatalytic hydrogen production by a Ga(III) complex in water. **A. Arnold**, L.A. Berben

9:30 INOR **80.** Self-assembly processes: Connected spherical nano-sized supramolecules. **B. Krämer**, M. Scheer

9:50 INOR **81.** Host-guest systems: Encapsulation of various templates by self-assembled supramolecules. **H. Brake**, M. Scheer

10:10 Intermission.

10:20 INOR **82.** X-ray and neutron scattering study of the formation of giant molecular metal oxide clusters. **P. Yin**

10:40 INOR **83.** Cobalt supramolecular triple-stranded helicate-based discrete molecular cage. **H. Yoo**

11:00 INOR **84.** Synthesis, structure, and substitution reactivity of trinuclear molybdenum cluster compounds. **J.R. Houston**

11:20 INOR **85.** Accessing a copper(III)-alkylperoxo complex. **B.D. Neisen**, D. Dhar, N.L. Gagnon, W.B. Tolman

11:40 INOR **86.** Enhanced magnetic anisotropy and single-molecule magnet behavior in tetranuclear clusters featuring low-coordinate cobalt centers. **K. Chakarawet**, P. Bunting, J.R. Long

Section K

Moscone Center

3001

Lanthanide & Actinide Chemistry

Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

B. E. Cohen, L. Doerrer, J. Monteiro, *Presiding*

8:30 INOR **87.** Comparing molecular and band-based approaches to the antenna effect in lanthanide coordination polymers. **J. Einkauf**, D.T. de Lill

8:50 INOR **88.** Thiophene-based lanthanide complexes as photosensitizers for singlet oxygen generation. **M.A. Gracia-Nava**, A. De Bettencourt Dias

9:10 INOR **89.** Broadband porphyrin dyes for near-infrared emission of lanthanide ions. R.W. Arachchi, A. Kukoyi, **H. He**

9:30 INOR **90.** Lanthanide complexes of fluorinated alkoxide ligands. J. Weber, C. Kotyk, A.T. Royappa, A.L. Rheingold, **L. Doerrer**

9:50 Intermission.

10:00 INOR **91.** Lanthanide-doped nanocrystals engineered for low fluence multiphoton imaging. **B.E. Cohen**, B. Tan, A. Fernandez-Bravo, E. Chan, P. Schuck

10:20 INOR **92.** Template-directed synthesis of actinide nanoparticles. **A. Herve**, A. Braun, S. Alayoglu, C. Booth, D. Olive, M. Straub, S.G. Minasian

10:40 INOR **93.** Challenges in the design of luminescent markers and cation sensors based on lanthanide complexes. **J. Monteiro**, D. Tapia, A. De Bettencourt Dias

11:00 INOR **94.** Comparison of Li with K and Na in rare-earth metal reduction chemistry: Isolation of $[Li(2.2.2\text{-cryptand})]^+$ in unique coordination environments. **D.N. Huh**, J.W. Ziller, W.J. Evans

11:20 Intermission.

11:30 INOR **95.** New vistas in organometallic actinide chemistry. **J.K. Pagano**, K. Erickson, J. Xie, D.E. Morris, B. Scott, R. Wu, L. Gagliardi, R. Waterman, J.L. Kiplinger

11:50 INOR **96.** Investigations of the electronic structure of actinide-aluminum bimetallics: Synthesis, reactivity and XAS characterization of actinide-alanate molecules and other actinide-aluminum materials. **A.B. Altman**, A. Brown, J. Arnold, S.G. Minasian, S. Pemmaraju, D. Prendergast, D.K. Shuh, T. Tyliszczak, D. Vine

12:10 INOR **97.** Synthesis and reactivity of a homoleptic uranium(III) tris(aryl) complex. **M. Boreen**, B. Parker, T.D. Lohrey, J. Arnold

Section L

Moscone Center

3003

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

A. Poater, *Presiding*

8:30 INOR **98.** Evolution of reactivity of olefin metathesis of Ru, and a step forward to other metals. **A. Poater**

8:50 INOR **99.** Ruthenium-based olefin metathesis: Insight into catalyst decomposition. **G.G. Lavoie**, T.G. Larocque, A.C. Badaj

9:10 INOR **100.** Synthesis, structure and characterization of new ruthenium(II) complexes and their catalytic activities towards selective C-O bond formation via activation of terminal alkynes. **R.K. Jena**, M. Bhattacharjee

9:30 INOR **101.** Catalytic upgrading of ethanol to butanol: Mechanistic insights. **H. Aitchison**, D. Wass, R. Wingad

9:50 INOR **102.** CO_2 and formic acid, a winning couple in reduction chemistry. **T. Cantat**

10:10 INOR **103.** Mechanistic studies of oxidative arene vinylation catalyzed by late transition metals. **B.A. Vaughan**, S.K. Khani, J.B. Gary, J.D. Kammert, J. Chen, M.S. Webster-Gardiner, B.A. McKeown, R.J. Davis, T.R. Cundari, T.B. Gunnoe

‡ *Cooperative Cosponsorship*

10:30 INOR **104.** Mechanistic study of thermal oxidative addition of si-h bond to mixed n-heterocylic carbene oxazolinylborato rhodium bis(carbonyl) complex. **A. Biswas**

10:50 INOR **105.** Cationic rhenium(III) complexes: Synthesis, characterization, and reactivity for catalytic hydrosilylation of aldehydes. **D.E. Perez**, E.A. Ison

11:10 INOR **106.** Rh-catalyzed C-H cyanation of imidazopyridine using N-cyano-N-phenyl-p-methylbenzenesulfonamide as the cyano source. X. Shen, J. Qu, C. Liu, Y. Guo, **X. Zhu**, X. Hao, M. Song

11:30 INOR **107.** Mechanistic studies of Rh(diphosphine)-catalyzed methanol reductive carbonylation. **S. Chotchatchawankul**, C.R. Landis

Section M

Moscone Center

2000

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

R. Blanski, D. Mendoza-Espinosa, *Presiding*

8:30 INOR **108.** Bicyclic (alkyl)(amino)carbenes (BicAACs): Introducing the first of a new family of stable carbenes. **E. Tomas Gonzalez de Mendivil**, M.M. Hansmann, R. Jazzar, M. Melaimi, G. Bertrand

8:50 INOR **109.** Imidazolin-2-ylidenaminophosphines: A highly electron-rich phosphorus(III) superbase that splits CO_2. **P. Mehlmann**, F. Dielmann

9:10 INOR **110.** Withdrawn.

9:30 INOR **111.** New class of N-heterocyclic carbenes featuring closo-carborane anions. **S. Lee**, V. Lavallo

9:50 INOR **112.** Highly functionalized N-heterocyclic carbenes bearing icosahedral carborane anions. **S.G. McArthur**

10:10 INOR **113.** Chiral acyclic diaminocarbene gold complexes as catalysts for enantioselective intramolecular hydroamination of allenes: Systematic study of ligand substituent effects on enantioselectivities. **A. Ruch**, V. Nesterov, L.M. Slaughter

10:30 Intermission.

10:40 INOR **114.** Synthesis of back-functionalized imidazolinium salts and NHC carbene complexes. **R. Blanski**, H. Phan, R.H. Grubbs

11:00 INOR **115.** Novel phosphine ligand with NH linker for ligand cooperative catalysis. **K. Ding**, L. Alhthlol, D. Tyer, S. Xu

11:20 INOR **116.** Mono/di/triphosphine complexes of transition metals based on tris(3-methyl-1H-indol-2-yl) methane as a model system for the study of apical metal–H–C_{sp3} interactions. **E. Smirnova**, J. Lloret-Fillol

11:40 INOR **117.** Synthesis of Co and Mo hydroxycyclopentadienyl complexes and their catalytic activities in transfer hydrogenation. **W. Wu**, R.M. Waymouth, T. Seki, D. Solis, K. Nozaki, H. Ando, S. Kusumoto

12:00 INOR **118.** P-P bond formation via unique metal-ligand cooperation. **Y. Kim**, Y. Lee

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Sponsored by PHYS, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis, & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Synthesis of Catalysts by Non-Traditional Methods

Nanoparticle Catalysts

Sponsored by CATL, Cosponsored by COLL and INOR

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

SUNDAY AFTERNOON

Section A

Moscone Center

2009

Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator: Symposium in honor of Nilay Hazari

W. H. Bernskoetter, A. Valentine, *Organizers*

A. Hazari, *Presiding*

1:30 INOR **119.** Operando NMR studies of hydroformylation. **C.R. Landis**, A. Brezny

1:55 INOR **120.** Lewis acid additives in organotransition metal chemistry. **G. Dobereiner**

2:20 INOR **121.** Gold(III) catalyst design for alkene and alkyne functionalization reactions. **A. Nova**

2:45 Intermission.

2:55 INOR **122.** Lewis acid-transition metal protomoed carbon dioxide functionalization. **W.H. Bernskoetter**, D. Jin

3:20 INOR **123.** Proton-Assisted Reduction of CO2 by Cobalt Aminopyridine Complexes. **S.C. Marinescu**, A. Chapovetsky

3:45 INOR **124.** Catalytic hydrogenolysis of carbon oxygen bonds. **D.M. Heinekey**, K.I. Goldberg, J.M. Goldberg, L.M. Guard, T. Lekich

4:10 INOR **125.** Molecular catalysts for water oxidation. **G.W. Brudvig**, R.H. Crabtree, S.B. Sinha, D.Y. Shopov, L.S. Sharninghausen, T. Michaelos, H. Lant, K. Fisher

Section B

Moscone Center

2011

Celebrating 60 Years of the Division of Inorganic Chemistry

The Next Decades: 1990's & 2000's

M. J. Clarke, D. C. Crans, *Organizers*

B. E. Bursten, S. Ronco, M. Scott, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **126.** From siderophores to supermolecules, fifty years of coordination chemistry. **K.N. Raymond**

2:05 INOR **127.** Electrochemically-promoted catalytic asymmetric hydrogenation using chiral organorhodium complexes. **B.T. Donovan-Merkert**

2:35 INOR **128.** Solid state chemistry, Zintl phases, and the Division of Inorganic Chemistry. **S. Kauzlarich**

3:05 INOR **129.** Surface chemistry of II-VI nanoplatelets and nanoribbons. Y. Zhou, Y. Yao, C. Morrison, **W.E. Buhro**

3:35 Intermission.

3:50 INOR **130.** Antimony(V) Lewis acids: Applications in anion sensing and small molecule activation. **F.P. Gabbai**

4:20 INOR **131.** Metalloprotein design: Examination of mononuclear redox centers. **V.L. Pecoraro**, A. Tebo, K. Koebke

4:50 INOR **132.** Synthesis of new bismuth based materials. J. Walsh, S.M. Clarke, **D.E. Freedman**

5:20 INOR **133.** Celebrating 60 Years - Inorganic chemistry at the National Science Foundation. **C.A. Bessel**

Section C

Moscone Center

2016

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

A. Johnson, *Presiding*

1:30 INOR **134.** Synthesis and reactivity of compounds containing a κ^3-1,1′-bis(diphenylphosphino) ferrocene ligand. **K. Cabrera**, C. Nataro

1:50 INOR **135.** Synthesis and characterization of antimony(V) Lewis Acids. **N. Capra**, A.M. Christianson, F.P. Gabbai

2:10 INOR **136.** Heterogeneous and homogeneous phosphonothioate alcoholysis by supported molybdenum-peroxo complexes. **L.Y. Kuo**, A. Bennett

2:30 INOR **137.** Evaluating the role of linker flexibility in base-free transfer hydrogenation of aldehydes and ketones catalyzed by Cp*Ir(pyridinesulfonamide)Cl complexes. **T.M. Townsend**, A.R. O'Connor

2:50 INOR **138.** Alkane functionalization with (^{dm}phebox)Ir$(OAc)_2(OH_2)$. **Z.H. Syed**, A.M. Wright, S.B. Rubashkin, K.I. Goldberg

3:10 Intermission.

3:25 INOR **139.** Group VI metal complexes of tris(diisopropylphosphinomethyl)phenylborate. **P.J. Fischer**, S. Senthil, J.T. Stephan, M.D. Storlie, M.L. Swift, V.G. Young, Jr.

3:45 INOR **140.** Reactivity of titanium-aluminum heterobimetallics. **A. Brown**, A.B. Altman, S. Hohloch, T.D. Lohrey, S.G. Minasian, J. Arnold

4:05 INOR **141.** Palladium complexes of amine bis(phenolate) ligands: Complex isolation and catalytic evaluation. E. Collins, B.J. Graziano, A.K. Bowser, **B. Wile**

4:25 INOR **142.** Synthesis, reactivity, and catalytic applications of isolable NHC-CuCF2H complexes. **S. Kariofillis**, J.R. Bour, M.S. Sanford

Section D

Moscone Center

2018

ACS Award in Inorganic Chemistry: Symposium in honor of Lawrence Que, Jr.

M. J. Maroney, *Organizer*

E. L. Que, *Organizer, Presiding*

F. Li, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **143.** Rational design of biologically inspired catalysts for selective oxidation reactions. **M. Costas**, J. Serrano Plana, O. Cussó, A. Company, M. Milan

2:00 INOR **144.** Biomimetic metal-oxygen intermediates in dioxygen activation chemistry. **W. Nam**

2:25 INOR **145.** Spectroscopic, and/or crystallographic characterization of metastable intermediates involved in cysteinate-ligated non-heme iron-promoted reaction mechanisms. M.N. Blakely, M.A. Dedushko, A.S. Ganas, G. Villar-Acevedo, P. Lugo-Mas, **J. Kovacs**

2:50 INOR **146.** High valent metal oxo and nitrene cores in chemistry and biology. **K. Ray**

3:15 Intermission.

3:30 INOR **147.** Catching transient intermediates in non-heme iron oxidation chemistry with high speed Raman spectroscopy. D. Unjaroen, S. Padamati, J. Chen, A. Draksharapu, M. Swart, **W.R. Browne**

3:55 INOR **148.** Insights into metalloenzyme function from bio-inspired manganese complexes. **T.A. Jackson**, D. Rice, A.A. Massie, M. Denler

4:20 INOR **149.** Tuning the reactivity of high-valent nickel-oxygen adducts for hydrocarbon oxidation. **A.R. McDonald**

4:40 INOR **150.** Relationship between electronic structure and reactivity in nonheme dioxygenase models. **A.T. Fiedler**, A.A. Fischer, S.V. Lindeman

5:00 INOR **151.** Spectroscopic studies and oxidizing reactivity of two high-valent nickel-oxygen species. T. Corona, A. Draksharapu, S. Padamati, F.F. Pfaff, F. Acuña-Parés, V. Martin-Diaconescu, J. Lloret Fillol, K. Ray, **A. Company**

Section E

Moscone Center

2020

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

K. R. Kittilstved, E. J. McLaurin, *Organizers*

R. Beaulac, *Presiding*

1:30 INOR **152.** Correlating structure and function in symmetric and asymmetric core/shell optical nanomaterials. **J.A. Hollingsworth**

2:00 INOR **153.** Understanding localized surface plasmon resonance in doped metal oxide nanocrystals. **D.J. Milliron**

2:30 INOR **154.** Controlling dopant-defect interactions in doped $SrTiO_3$ colloidal nanocrystals. **K.R. Kittilstved**

3:00 Intermission.

3:15 INOR **155.** Enhanced Multiple Exciton Generation in PbS/CdS Janus-like Heterostructure Nanocrystals. D. Kroupa, G. Pach, B. Chernomordik, **M.C. Beard**

3:45 INOR **156.** Sample-Transmitted Excitation Photoluminescence (STEP) technique for quantifying the energy flow in nanocrystals and their solids. **M. Zamkov**

4:15 INOR **157.** Optical Stark metrology of CdSe nanocrystal quantum dots: On the size-dependence of the oscillator strength. Y. Tang, M. Saniepay, C. Mi, R. Beaulac, **J. McGuire**

Section F

Moscone Center

2022

Sustainability in Electrocatalytic Fuel & Chemical Production

Cosponsored by CATL

L. A. Berben, J. L. Dempsey, *Organizers*

E. S. Wiedner, *Presiding*

1:30 INOR **158.** Use of polyoxometalates as redox-active resevoirs: Towards small molecule activation. **E.M. Matson**

1:55 INOR **159.** Studies of electrocatalytic dioxygen reduction. **J.M. Mayer**, M.L. Pegis, C. Wise, D.J. Martin, S. Raugei, N. Kumar

2:20 INOR **160.** Observing molecular vibrations of catalytic intermediates at electrode surfaces. **T. Cuk**, S. Pemmaraju, D. Prendergast, X. Chen, M. Waegele, D. Herlihy

2:45 Intermission.

3:00 INOR **161.** Hydricity as an activity descriptor for molecular hydrogen evolution electrocatalysts. C. Tsay, B. Ceballos, D. Cunningham, S. Ruelas, **J.Y. Yang**

3:25 INOR **162.** Solar fuel devices with molecular catalysts – mechanistic insights. **L. Hammarstrom**

3:50 INOR **163.** Designing small molecule electrocatalysts for selective C-H bond formation with CO_2: $[Fe_4N(CO)_{12}]^-$, $[Fe_4N(CO)_{12}]^{2-}$, and the role of the hydride intermediate, $[H\text{-}Fe_4N(CO)_{12}]^-$ in catalysis. N.D. Loewen, A. Taheri, **L.A. Berben**

4:15 INOR **164.** CO2 splitting into CO and O2 : From mechanistic studies to efficient electrolyzer. **C. Cyrille**

Section G

Moscone Center

2024

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

X. Bu, P. Yang, D. Zhao, N. Zheng, *Organizers*

Q. Zhang, *Organizer, Presiding*

1:30 INOR **165.** Hybrid nanomaterials for treating resistant cancers. **W. Lin**

1:50 INOR **166.** Dynamic metal–organic frameworks: Design and properties. **X. Bu**

2:10 INOR **167.** Oxygen evolution reaction electrocatalysis: Redefining intrinsic activity trends and illustrating design principles. **S.W. Boettcher**

2:30 INOR **168.** Towards robust hierarchical porous metal–organic frameworks. S. Yuan, **H. Zhou**

2:50 INOR **169.** Porous ionic liquids: Challenges and opportunities. **S. Dai**

3:10 Intermission.

3:40 INOR **170.** Organometallic chemistry of macrocycles, cages. **G. Jin**

4:00 INOR **171.** Metal-Organic Frameworks (MOFs): Platforms for multifunctional materials. **B. Chen**

4:20 INOR **172.** Luminescent coordination networks: Structure, functionality and applications. W. Liu, W.P. Lustig, Y. Fang, K. Zhu, **J. Li**

4:40 INOR **173.** Development of metal-organic frameworks as a versatile platform for heterogeneous catalysis. **S. Ma**

Section H

Moscone Center

3000

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Cosponsored by BIOL

Financially supported by Northwestern U, U of California-Davis

V. DeRose, *Organizer*

J. A. Telser, *Organizer, Presiding*

1:30 INOR **174.** High resolution x-ray spectroscopic studies of soluble methane monooxygenase. **S. DeBeer**

2:00 INOR **175.** Mechanism and control in radical SAM enzymes. **J.B. Broderick**, M. Horitani, A.S. Byer, K.A. Shisler, T. Chandra, R.U. Hutchison, K.S. Duschene, A.R. Marts, W.E. Broderick, B.M. Hoffman

2:30 INOR **176.** Structure of a heme peroxidase compound II. H. Kwon, J. Basran, A.J. Fielding, T.E. Schrader, A. Ostermann, M.P. Blakeley, P.C. Moody, **E. Raven**

3:00 INOR **177.** Vibrational studies of the single turnover reaction cycle and substrate inhibition reaction in denitrifying NO reductases. **P. Moënne-Loccoz**

3:20 Intermission.

3:30 INOR **178.** Effects of heme conformation on spin state, spin distribution, and electron transfer in cytochromes. **K. Bren**, J. Kleingardner, B. Kandemir

4:00 INOR **179.** Using biosynthetic models of heteronuclear metalloenzymes for spectroscopic elucidation of their mechanisms in multi-electron processes. **Y. Lu**, A. Bhagi-Damodaran, C. Cui, Y. Yu, J. Reed

4:20 INOR **180.** Developing protein-based model systems to mimic hydrogenase, carbon monoxide dehydrogenase, and acetyl coenzyme A synthase. **H.S. Shafaat**, J.W. Slater, C.R. Schneider, A. Manesis, S.C. Marguet, M.J. Stevenson

4:40 INOR **181.** Biosynthesis of the [FeFe]-hydrogenase active site. **D. Suess**

5:00 INOR **182.** Nitrogen fixation by nitrogenase: The heart of the mechanism. **B.M. Hoffman**

Section I

Moscone Center

3010

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Homogeneous Catalysis

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREM, Argonne National Lab, Northwestern University

A. Facchetti, *Organizer*

T. Lohr, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR **183.** Design and synthesis of phosphine-olefin ligands with planar-chiral metal complex scaffold and application in asymmetric catalysis. **M. Ogasawara**

2:05 INOR **184.** Late stage functionalization of bioactive natural products under catalyst control. **M.R. Gagne**

2:35 INOR **185.** Development of cooperative asymmetric catalysts. **S. Hong**

3:05 Intermission.

3:15 INOR **186.** Catalytic challenges in organoactinide chemistry. **M.S. Eisen**

3:45 INOR **187.** Chemical transformation of dinitrogen mediated by pincer complexes. **S. Schneider**

4:15 INOR **188.** Transition-metal-catalyzed functionalization using carbon dioxide. **Y. Tsuji**

Section J

Moscone Center

3012

ACS Award in Organometallic Chemistry: Symposium in honor of Marcetta Y. Darensbourg

C. G. Riordan, *Organizer*

D. Mason, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR **189.** Insights into the catalytic mechanisms of [FeFe] hydrogenase: Inspiration for the design of molecular catalysts. **W. Lubitz**, A. Adamska-Venkatesh, J.A. Birrell, C. Sommer, S. Rumpel, O. Rudiger, E. Reijerse

2:00 INOR **190.** Control of the activity of [FeFe]-subsite analogues by interactions of their ligated cyanides. **C. Pickett**, J. Woods

2:25 INOR **191.** Effect of the dithiolate cofactor on the reactivity, spectroscopy, and electrochemistry of models for the [FeFe]-hydrogenases. **T.B. Rauchfuss**, N. Lalaoui, C.P. Richers, M.R. Carlson, W. Wang

2:50 INOR **192.** Computational modeling of hydrogenases and biomimetic complexes. **M.B. Hall**

3:15 INOR **193.** Effect of the outer coordination sphere on molecular catalysts: A tribute to Marcetta, the hydrogenase whisperer. **W.J. Shaw**, N. Boralugodage, A. Dutta, B. Ginovska, S. Raugei

3:40 Intermission.

3:55 INOR **194.** Solar fuels science. **H.B. Gray**

4:20 INOR **195.** Hydrogen evolution without metal-hydrides: Ligand-centered HER catalysts with transition metals and non-transition metals. **C.A. Grapperhaus**, A.Z. Haddad, B. Garabato, R.M. Buchanan, P.M. Kozlowski

4:45 INOR **196.** Pyridine and pyrazine pincer coordination chemistry. **K. Bowman-James**

5:10 INOR **197.** Redox-active ligand complexes in artificial photosynthesis and the reductive side of water splitting. **R. Eisenberg**, G. Li

Section K

Moscone Center

3001

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

I. Kim, T. Runcevski, *Presiding*

1:30 INOR **198.** Effect of different synthesis methods and strategies on the properties of copper based and iron based metal organic frameworks. **A. Yurdusen**, Y. Yurum

1:50 INOR **199.** Redox active metal-organic frameworks with multi-components in order. B. Tu, **Q. Li**

2:10 INOR **200.** Withdrawn.

2:30 INOR **201.** *In Situ* diffraction and spectroscopic studies of metal-organic frameworks under variable temperature and gas pressure. **T. Runcevski**, J.R. Long

2:50 INOR **202.** Coordination polymers featuring coordinatively unsaturated, low-valent metal centers. **D.W. Agnew**, J.S. Figueroa

3:10 INOR **203.** General interfacial synthesis route to free-standing metal-organic framework membrane. **Z. Li**, W. Han, K. Yeung

3:30 Intermission.

3:45 INOR **204.** Self-assembled coordination polymer as intermediate in synthesis of porous oxide from bulk metal. **B. Chang**, J. Chen, I. Tevis, S. Cinar, S. Oyola-Reynoso, G. Rodriguez, A.J. Rossini, M. Thuo

4:05 INOR **205.** Phosphine and arsine coordination materials with well-defined open metal sites: New examples with Pd(II) and Au(I). **S.M. Humphrey**, S.G. Dunning, E. Sikma, J. He

4:25 INOR **206.** POMOFs and POMzites: A family of zeolitic polyoxometalate frameworks from a minimal building block library. **L. Cronin**

4:45 INOR **207.** Coordinative alignment of molecules in chiral metal organic frameworks structure determination of molecules coordinated and aligned in MOFs by single crystal x-ray diffraction. **S. Lee**, E.A. Kapustin, O.M. Yaghi

5:05 INOR **208.** Nanocasting in metal-organic framework materials. **A. Stein**, C. Malonzo, Z. Wang, W. Zhao, T.E. Webber, R. Penn

5:25 INOR **209.** Nomenclature, terminology guidelines, and database issues for topology representations in metal-organic frameworks. **L.R. Ohrstrom**

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

Section L

Moscone Center
3003

Inorganic Catalysts

S. A. Koch, *Organizer*

J. Bluemel, E. V. Rybak-Akimova, *Presiding*

1:30 INOR **210.** Mechanistic investigations of oxygen evolution at a manganese-doped cobalt cubane catalyst. **E. Darby**, A. Nguyen, S. Gul, J. Yano, T.D. Tilley

1:50 INOR **211.** Pt NPs ligated by zwitterionic imidazolium-amidinates: A notable ligand effect in hydrogenation of carbonyl groups. **L.M. Martínez-Prieto**, B. Chaudret, J. Campora, P.W. van Leeuwen

2:10 INOR **212.** Synthesis and characterization of tin (II) complexes supported by N_2O_2 bis(phenoxy)-amine ligands for the ring-opening polymerization of lactide. **S. Praban**, K. Phomphrai

2:30 INOR **213.** Computational study of the vanadium-catalyzed decomposition of alkyl hydroperoxides to ketones. **M. Hermsen**, A. Schmidt, A. Schäfer, T. Schaub

2:50 INOR **214.** Dizinc lactide polymerization catalysts: Hyperactivity by control of ligand conformation and metallic cooperativity. **A.A. Thevenon**, C. Romain, M. Bennington, H. Davidson, A. White, S. Brooker, C.K. Williams

3:10 Intermission.

3:20 INOR **215.** One-pot synthesis of double-capped oligoesters using simple metal amides. **P. Piromjitpong**, K. Phomphrai

3:40 INOR **216.** Mechanism for the oxidation of alcohols by a μ-oxido-diiron(III)bis-phenolato polypyridyl complex. **D. Unjaroen**, A. Draksharapu, M. Swart, W.R. Browne

4:00 INOR **217.** Towards inert C–H bond functionalization using main group multiple bonds. **J. Chu**, G. Menard

4:20 INOR **218.** Immobilized Sonogashira catalyst systems. **J. Bluemel**, J.C. Pope

4:40 INOR **219.** Kinetics and mechanisms of hydrocarbon oxidations with H_2O_2/HOAc catalyzed by iron and manganese complexes with rigid aminopyridine ligands. **E.V. Rybak-Akimova**, G. Yang, M. Piquette

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Theory & Modeling

Sponsored by PHYS, Cosponsored by INOR

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Synthesis of Catalysts by Non-Traditional Methods

Model Catalysts, Microporous Materials & Oxides

Sponsored by CATL, Cosponsored by COLL and INOR

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

SUNDAY EVENING

Section A

Moscone Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

5:30 - 7:30

INOR **220.** IONiC VIPEr workshops: Bringing current literature into the classroom. **S. Poland**, **B.B. Sears**, **S.A. Toledo**, **A.R. Johnson**

INOR **221.** IONiC bonding: Building a lattice using attractive forces. **A.R. Johnson**, **J.L. Stewart**, A.K. Bentley, H.J. Eppley, E.R. Jamieson, C. Nataro, B.A. Reisner, S.R. Smith, L.A. Watson, N. Williams

Section B

Moscone Center
Hall D

Celebrating 60 Years of the Division of Inorganic Chemistry

D. C. Crans, *Organizer*

5:30 - 7:30

INOR **222.** Highlights in inorganic chemistry from the 250 years that preceded the creation of the Division of Inorganic Chemistry. **S.A. Koch**

INOR **223.** Cobalt and copper σ-complexes with a diphosphine-hydrosilane ligand. J. Kim, Y. Kim, **Y. Lee**

INOR **224.** Trends in NMR chemical shifts of d^0 transition metal compounds. **Z. Xue**, T.M. Cook, A.C. Lamb

INOR **225.** Effect of confinement on the acidity of organic and bio ligands. **J. Salas**, A. Cherem, M.D. Johnson

INOR **226.** Selenium speciation in the Fountain Creek water and effects on fish species diversity. **J. Carsella**, S.J. Bonetti, D.C. Crans, S.J. Herrmann, D.R. Nimmo

INOR **227.** Ruthenium complexes as potential anticancer prodrugs that are activated by low pH and light. **J. Gray**, F. Qu, J.A. Lundeen, N.S. Chambers, J. Park, Y. Kim, J.J. Paul, E.J. Merino, R.H. Schmehl, E.T. Papish

INOR **228.** Group transfer and methylenation reactions of a terminally bound zirconium methylidene complex. **T. Kurogi**, P. Carroll, D.J. Mindiola

INOR **229.** Energy transfer from PbS nanocrystals to pentacene. **X. Li**, M. Tang

INOR **230.** Diaquo ruthenium water oxidation catalysts with a novel biimidazolyl backbone. **J.M. Kamdar**, C.E. Moore, A.L. Rheingold, D.K. Smith, D.B. Grotjahn

INOR **231.** Withdrawn.

INOR **232.** Withdrawn.

INOR **233.** Correlating redox potential with ^{51}V NMR chemical shifts for vanadium (V) catecholates. **J.T. Koehn**, P. Chatterjee, C.N. Beuning, A. Waterhouse, T. Lucia, T.E. Polenova, D.C. Crans

INOR **234.** Diverse array of nucleophilic reactivity featuring molecular titanium nitride complexes. **L. Grant**, P. Carroll, B. Manor, D.J. Mindiola

Section C

Moscone Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

5:30 - 7:30

INOR **235.** Iron and cadmium binding in metalloprotein II and myohemerythrin from *Hediste diversicolor*. **A. Krieger**, B. Russell

INOR **236.** Synthesis and evaluation of alkynyl β-sheet mimetics coordinated to tungsten. **E.C. Pedro**, A.N. Boynton, S.M. Berk, T.P. Curran

INOR **237.** Manganese corrole substituted myoglobin. **J.M. Mason**, K.L. Stone

INOR **238.** Investigating dechlorination using bio-inspired nickel compounds. **E. Gund**, R. Griffin, C. Ye, K.M. Van Heuvelen

INOR **239.** Copper (I) substitution at zinc (II) binding domains: Characterization of speciation and functional studies. **M.L. Stevens**, **M.D. Storlie**, K.E. Splan

INOR **240.** Preparation of synthetic conjugated myoglobin to promote new reactivity. **K.L. Stone**, J. Hua, H. Choudhry, J. Mason

INOR **241.** Tandem C-H functionalizations by combining light-driven biocatalysis and photocatalysis. **V. Alfaro**, **J. Faris**, **M. Melkie**, C. Sulca, T. Banh, M. Kato, L.E. Cheruzel

INOR **242.** Synthesis, characterization and photosensitization in a series of $Ru(phen)_2(quo)]^+$ complexes. **F. Delano IV**, A. Koerner, A. Cardillo, R.N. Garner, B.B. Sears

INOR **243.** Synthesis and investigation of novel hydroquinone ring-cleaving dioxygenase model complexes. **N. Porter**, T.E. Machonkin, A. Speelman, P.L. Holland

INOR **244.** Copper binding and reactivity of de novo designed Due Ferri single chain (DFsc) proteins. **B. Van Dyke**, A.J. Reig

INOR **245.** Biophysical characterization and catalytic reactivity of rubrerythrin and symerythrin model proteins. **J. Pellegrino**, **K.A. Bell**, R. Polinski, S. Cimerol, A. Jacobs, E.I. Solomon, A.J. Reig

INOR **246.** Using model proteins to understand the structure-function relationships in 4-histidine/2-carboxylate diiron proteins. **C. Philip**, S. Hawkins, A.J. Reig

INOR **247.** Structure-function relationships in G4DFsc variants containing a 4-His/3-carboxylate active site. **K. OShea**, **J. Dorsheimer**, K. Biernat, A. Jacobs, E.I. Solomon, Y. Wu, W.F. Degrado, A.J. Reig

INOR **248.** Characterization of MnpC, a novel hydroquinone ring-cleaving dioxygenase. **J. Duncan**, E. Altman, T.E. Machonkin

INOR **249.** Molybdenum pyranopterin dithiolene complexes: Synthetic model and investigation in the role of pterin reduction in the molybdenum cofactor. **N. Nguyen**, **B. Williams**, **D. Gisewhite**, **S.J. Nieter Burgmayer**

INOR **250.** Mechanistic investigation of photochemical products from iron-iron hydrogenase model compounds. P. De La Torre, A. Nelson, **C.F. Works**

INOR **251.** Synthesis and characterization of cobalt (II) salen and its possible interactions with persulfide species. A. Holm, V. Suarez, L. Alvarez, **C.F. Works**, J. Fukuto

INOR **252.** Dechlorination abilities of biomimetic compounds. **C. Ye**, R. Griffin, K.M. Van Heuvelen

INOR **253.** Investigating the reactivity of the ligating histidines at the Cu_A site of cytochrome c oxidase. **T. Devlin**, L.M. Hunsicker Wang

INOR **254.** Changes in reduction potential of the [2Fe-2S] cluster of the *Thermus thermophilus* Rieske protein using multiple non-covalent interactions. **R. Shepherd**, L.M. Hunsicker Wang

INOR **255.** Exploring the effect of distal charges on the reduction potential of the Rieske protein from *Thermus thermophilus*. **M. Hogsett**, **J. Munoz**, L.M. Hunsicker Wang

INOR **256.** Metal-organic supercontainers for neurobiological applications. **J.W. Fanta**, Z. Wang, B. Burrell

INOR **257.** Mechanistic investigation of the solvent dependent photochemistry of iron-iron hydrogenase model compounds. B. Jolly, L. Ortiz, **C.F. Works**

INOR **258.** Studying the active site of nickel-acireductone dioxygenase through nickel and zinc analogues: A structural and spectroscopic comparison study. **A.J. Gremillion**, S. Sanchez, S.A. Toledo, V. Lynch, C.L. Dorsey

INOR **259.** Capturing an intermediate of the radical *S*-adenosyl-L-methionine enzyme lysine 2,3-aminomutase. **C. Denler**, A.S. Byer, J.B. Broderick

Section D

Moscone Center
Hall D

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of William B. Tolman

L. M. Berreau, P. L. Holland, *Organizers*

5:30 - 7:30

INOR **260.** Characterization of a copper(III)-phenoxide complex. **N.L. Gagnon**, D. Dhar, W.B. Tolman

INOR **261.** Probing the effect of ligand electronics on the C-H reactivity of copper-oxygen cores. **C. Elwell**, W.B. Tolman

INOR **262.** Analysis of novel tetradentate zinc catalysts used for the polymerization of rac-lactide. **A.M. Luke**, D.E. Stasiw, T. Rosen, M. Kol, W.B. Tolman

INOR **263.** New strategy for the hydroxylation of strong C-H bonds. **H. Sajjad**, W.B. Tolman

INOR **264.** Mechanistic analysis of the alternating copolymerization of epoxides with cyclic anhydrides utilizing a cocatalyst system. **L.A. Mitchell**, M. Fieser, D. Urness, M.J. Sanford, C.R. Dunbar, M. Mandal, C.J. Cramer, G.W. Coates, W.B. Tolman

INOR **265.** Resonance Raman spectroscopy of copper(III)-hydroxide core and structural implications based on a unified Badger's rule. **A.D. Spaeth**, N.L. Gagnon, W.B. Tolman

INOR **266.** Mechanistic studies of ε-caprolactone polymerization by (salen)AlOR complexes and a predictive model for cyclic ester polymerizations. **J.A. Macaranas**, A.M. Luke, E.E. Marlier, M. Mandal, D. Marell, C.R. Dunbar, M. Johnson, Y.C. DePorre, M.O. Miranda, B.D. Neisen, C.J. Cramer, M.A. Hillmyer, W.B. Tolman

Section E

Moscone Center

Hall D

ACS Award in Inorganic Chemistry: Symposium in honor of Lawrence Que, Jr.

M. J. Maroney, E. L. Que, *Organizers*

5:30 - 7:30

INOR **267.** Green synthesis of Nd-La doped $Sr_2Cu_2Fe_{28}O_{46}$ and Nd-La doped $Sr_2Mg_2Fe_{28}O_{46}$ nanoparticles and comparison their magnetic and microwave absorbing properties with Nd-La doped $Sr_2CuMgFe_{28}O_{46}$ nanoparticles. **P. Alimard**

INOR **268.** Characterization of (μ-oxo) heterobimetallic complexes derived from [Fe^{IV}(O)TMC] with Fe coordination numbers that depend on ligand topology. **A. Zhou**, J. Prakash, G. Rohde, J. Klein, S.T. Kleespies, A. Draksharapu, R. Fan, Y. Guo, C.J. Cramer, L. Que

INOR **269.** Tuning the C—H bond cleavage ability of an oxoiron(IV) complex structural properties of an oxoiron(IV) complex supported by a pentadentate ligand. **W. Rasheed**, M. Puri, A. Draksharapu, L. Que

INOR **270.** Inner side of high-valent metal-oxo reactivity. **M. Swart**, K. Ray

INOR **271.** Exploring the H_2O_2 interaction and catalytic activity of mononuclear Cu (II) coordination complexes containing N-rich ligand architecture. **N. Singh**, J. Niklas, O. Poluektov, K.M. Van Heuvelen, A. Mukherjee

INOR **272.** Two isomers of oxoiron(IV) complex supported by tetramethylcyclam ligand: Interconversion and reactivity. **J. Prakash**, J. Klein, A. Draksharapu, C.J. Cramer, L. Que

INOR **273.** Reversible formation an Fe^{III}–O–Ce^{IV} intermediate from the reaction of Fe^{IV}=O and Ce^{III}. **A. Draksharapu**, J. Klein, W. Rasheed, C.J. Cramer, L. Que

INOR **274.** Factors influencing the electronic nature of the active oxidant in a bio-inspired non-heme mononuclear iron catalyst. **S. Kal**, S. Iyer, L. Que

INOR **275.** Modulation of a weakly coupled peroxo-dicopper(II) complex by interation with alkali metal ions. **L. D'Amore**, M. Swart, A. Brinkmeier, F. Meyer

INOR **276.** Characterization of a novel Fe(V)=O species using Mossbauer spectroscopy and Electron Paramagnetic Resonance (EPR) spectroscopy. **R. Fan**, J. Serrano Plana, A. Company, W.N. Oloo, L.A. Rueda, K.K. Meier, B. Verdejo, E.V. Garcia-Espana, M.G. Basallote, E.L. Bominaar, Y. Guo, L. Que, M. Costas, E. Munck

INOR **277.** Roles of (L)Fe^{V}(O) and (L)Fe^{III}–OOAc intermediates in bio-inspired C–H and C=C oxidations. Kinetics and spectroscopy. **W.N. Oloo**, R. Banerjee, S. Lee, C. Kim, J.D. Lipscomb, L. Que

INOR **278.** Elucidation of the mechanism of activation of oxygen by iron(II)polypyridylamine complexes in water. **D. Angelone**, J. Chen, A. Draksharapu, W.R. Browne, M. Swart

INOR **279.** Elucidation of high-valent species involved in carboxylic acid-assisted nonheme iron catalysis. **S. Xu**, A. Draksharapu, W. Ching, L. Que

INOR **280.** HDX-MS reveals metal-specific structural changes important to DNA binding by the cobalt and nickel responsive transcriptional regulator, RcnR. **H. Huang**, M.J. Maroney

INOR **281.** Role of citrate and transferrin in determining Ti(IV) solubility, bioavailability, and its regulation. **S. Sharma**

INOR **282.** Comparative reactivity studies of peroxomangaese(III) intermediates supported by two diazacycloalkane-based tetradentate ligands. **M. Denler**, T.A. Jackson, G. Wijeratne

INOR **283.** O-O bond activation by a series of Mn complexes supported by amide-containing ligands. **J. Parham**, G. Wijeratne, T.A. Jackson

INOR **284.** Metal-Assisted oxygen addition to an Fe(III)-thiolate. **M.N. Blakely**, G. Villar-Acevedo, M. Dedushko, W. Kaminsky, J. Kovacs

INOR **285.** InP based heterostructures: Synthesis, electronic structure, and quantitative comparison of absorption properties. **R. Toufanian**, M. Chern, A.M. Dennis

INOR **286.** Non-Covalent interactions in C-H oxidation reactions by metal-oxos: The curious case of CHD and DHA. **J. Klein**, B. Dereli, L. Que, C.J. Cramer

INOR **287.** Exploring the structure-reactivity relationship of a series of N5-ligated oxomanganese (IV) complexes. **A.A. Massie**, M. Denler, T.A. Jackson

INOR **288.** Tuning the proton-coupled electron-transfer reactivity of Mn(III)-hydroxo complexes via ligand perturbations. **D. Rice**, A. Burr, T.A. Jackson

INOR **289.** Thermodynamics of reactivity of a series of hydroxo-manganese complexes in H atom abstraction. **A. Munasinghe**, D. Rice, J. Parham, T.A. Jackson

INOR **290.** Withdrawn.

Section F

Moscone Center

Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Coordination Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

5:30 - 7:30

INOR **291.** Green chemistry in the advanced inorganic laboratory: Mechanochemical synthesis and characterization of homoleptic bis-chelate copper(I) complexes. **D.J. Rabaey**, **D.E. Janzen**

INOR **292.** Synthesis and kinetic studies of a trinuclear tungsten metal cluster. **J. Nunez**, R.C. Brookins, J.R. Houston

INOR **293.** Modifying the bridging anion of LnX_4M 12-metellacrown-4 complexes. **J.J. Reed**, J.C. Lutter, C.I. Daly, C. Chow, A.H. Davis, A. Nimthong-Roldan, M. Zeller, J.W. Kampf, C.M. Zaleski, V.L. Pecoraro, T.T. Boron

INOR **294.** Synthesis of a family of chiral aminoalcohols as ligands for titanium and tantalum catalyzed asymmetric hydroamination. A.R. Johnson, **C.S. Abelson**

INOR **295.** Withdrawn.

INOR **296.** Unique crystalline composite displaying four primary zoning events in the solid state and based upon self-assembled coordination polymers. **S. Cornell**, **S.R. Seidel**

INOR **297.** Axial ligand interactions of cyclometallated Pd(II) complexes: Hemilabile oxathiacrowns vs inert but fluxional thiacrowns. **D.E. Janzen**, M.A. Bruening, A.A. Mamiya, D.A. da Silva Filho

INOR **298.** Synthesis and characterization of SNS pincer ligand precursors and corresponding zinc(II) and copper(II) complexes. J.R. Miecznikowski, **T. Ostrowski**, M. Siu, K.A. Bayne, N.A. Bernier

INOR **299.** Synthesis, characterization, and reactivity studies of iron dibromide complexes bearing para-substituted alpha-diimine ligands. **D. Soemardi**, S.M. Click, A. Beltran, K.A. Wheeler, H.M. Hoyt

INOR **300.** Boron Schiff-Base complexes as detectors for toxic levels of selenate in water. **J. Bennett**, L. Jefferies

INOR **301.** Synthesis of a lanthanide complex using $Eu(NO_3)_3$ $6H_2O$ with tripodal ligand 2-OHnaphthtren (tris[*N*-(2-hydroxynaphthalidene)-2-aminoethyl]amine). **J.M. Armen**, P.M. Smith

INOR **302.** Activating carbon dioxide using a cobalt complex supported by a macrocyclic tetraza ligand. **A. Amado**, F. Li, C. Dong

INOR **303.** Syntheses, characterization, and oxygen reactivity of three coordinate SNS pincer copper(I) pincer complexes. **J.R. Miecznikowski**, **M.R. Smith**, M. Siu, N.A. Bernier, J. Jasinski, E. Reinheimer

INOR **304.** Synthesis of a new cationic cobalt(III) coordination complex and its potential applications as an indole ring forming catalyst. R.M. Miller, H.P. Nash, **A. Morris**

INOR **305.** Synthesis of new Fe and Co PONOP/PNP complexes: Towards the development of a first-row Guerbet catalyst. **T.M. Townsend**, C.E. Hayes, R. Baker, W.D. Jones

INOR **306.** Excimer and exciplex formation involving $[Pt(bphen)CN_2]$ and Ag^+ in solution. **E.J. Rourk**, J.K. Nagle

INOR **307.** Synthesis of europium(III) silicates using microwave-assisted hydrothermal methods. **Z.J. Woessner**, P.M. Smith

INOR **308.** Natural oxidation state analysis: Principles and applications. M.K. Heili, M. Nathan, **J.S. D'Acchioli**

INOR **309.** Synthesis and reactivity of actinide guanidinate complexes. **A. Shiau**, N. Settineri, J. Arnold

INOR **310.** Ionothermal synthesis and characterization of two new iron thiophosphates: $[EMIM]_2[Fe(P_2S_6)_2]$ and [PMIM] $[FeP_7S_{16}]$. **S.R. Kang**, M.L. Major, **J.A. Cody**

INOR **311.** Synthesis and characterization of thermotropic copper(II) heteroleptic metallomesogens with 2-ethylhexanoate ligands. **A. Beltran**, T.W. Clayton

INOR **312.** Withdrawn.

INOR **313.** Withdrawn.

INOR **314.** Synthesis and characterization of hyper-coordinate silicon complexes. **K.J. Goosherst**, J.M. Fritsch

INOR **315.** Progress toward the synthesis of potential AIE-active silafluorene derivatives. H. Tracy, J.L. Mullin, C.M. Prudente, **W. Lin**

INOR **316.** Computational results of ADF modelling of AIE-active luminophores. H. Tracy, J.L. Mullin, C.M. Prudente, **T.w. Nelson**

INOR **317.** Spectral characterization of potential AIE-active diphenylsilafluorene derivatives. J.L. Mullin, H. Tracy, C.M. Prudente, **N. Mathewson**

INOR **318.** Withdrawn.

Section G

Moscone Center

Hall D

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

5:30 - 7:30

INOR **319.** Comparison of 2,2'-bipyridine and 1,10-phenanthroline ancillary ligands in ruthenium metal complexes containing the 4,4'-dihydroxy-2,2'-bipryidine ligand. **A.E. Kuhn**, D.J. Charboneau, M.J. Kasher, N.A. Piro, W.S. Kassel, T. Dudley, J.J. Paul

INOR **320.** Synthesis, structure and catalytic applications towards *Cis-β*-ruthenium-salen complexes. **C. Lee**, C. Che

INOR **321.** Synthesis of heterometallic 12-MC-4 complexes with ligand and countercation substitutions. **G. Van Trieste**, M. Zeller, C.M. Zaleski

INOR **322.** Synthesis and luminescent study of lanthanide aluminum metallacrowns and metallacryptands. **J. Travis**, M. Zeller, C.M. Zaleski

INOR **323.** Synthesis of novel mixed O, N, S donor ligands. **E. Jugovic**, C. Hamaker

INOR **324.** NMR characterization of Ln-Mn-Na 12-metallacrown-4 complexes. C. Atzeri, V. Marzaroli, M. Quaretti, J. Travis, L. Di Bari, **C.M. Zaleski**, M. Tegoni

INOR **325.** Reactivity trends dictated by structure that influence terminal ligand substitution of alkylidyne-capped trinuclear molybdenum (IV) clusters. **R.C. Brookins**, J.R. Houston

INOR **326.** Theoretical and experimental investigation of Zn4Sb3 doped with metal elements. **K. Tsang**, R. Vellaisamy, R. Li

INOR **327.** Synthesis and characterization of 1,3-diphenyl-6-aryl fulvene coordination complexes. **B.J. O'Connell**, S.K. Adas, G.J. Balaich, S.T. Iacono

INOR **328.** Iron (II) pyridinediimine complexes with Lewis acids in the secondary coordination sphere. **K.T. Burns**, M. Delgado, J.M. Ziegler, J.D. Gilbertson

INOR **329.** Binding modes of Ni-CO_2 adducts and their CO_2 activation. **C. Yoo**, Y. Kim, Y. Lee

INOR **330.** Copper(I/II) reconfiguration of ligand conformations: Amplification and control of helicity by a single atom and solvent. **X. Duan**, T.M. Albelda, J.W. Canary

‡ *Cooperative Cosponsorship*

INOR **331.** Effects of carrier ligands on cispaltin analog binding to cysteine and methionine. **A.C. Smith**, K. Williams

INOR **332.** Analysis of S-Au-P bonding in phosphine gold(I) polifluorothiolates: Backbonding and weak interactions. **G. Moreno-Alcantar**, J.M. Guevara-Vela, H. Torrens

INOR **333.** Synthesis and structural characterization of chelating dinitrosyl iron complexes. **O. Becerra**, L. Li

INOR **334.** Electron donor-acceptor properties of substituted pyridine ligands on *fac*-tricarbonylrhenium(I) systems. **J.R. Farrell**, G. Kerins, K.L. Niederhoffer, L.A. Crandall, C.J. Ziegler

INOR **335.** Withdrawn.

INOR **336.** Synthesis and characterization of multinuclear manganese carboxylate coordination compounds by incorporating the anion of 3-(dimethylamino)-1,2- propanediol. **M. Reagan**, A. Saha

INOR **337.** Synthesis and characterization of novel sulfonamide ligands. **A. Penn**, C. Hamaker

INOR **338.** Syntheses, structures, and electrochemical studies of N,N'-bis(alkylthiocarbamate) butane-2,3-diimine Cu(II) complexes as pendant alkoxy derivatives of Cu(ATSM). **N.S. Vishnosky**, M.S. Mashuta, R.M. Buchanan, C.A. Grapperhaus

INOR **339.** Interactions between metal ions and ferrocenoyl-histidine peptide conjugates. **A. Ferranco**, H. Kraatz

INOR **340.** Synthetic control of coincidental formation of N-heterocyclic carbene-copper(I) complex within 2D and 3D metal-organic frameworks. **H. Lee**, K. Kim, E. Lee

INOR **341.** Withdrawn.

INOR **342.** Withdrawn.

INOR **343.** Synthesis and characterization of transition metal complexes with cyclic boraguanidinates. **C.M. Donahue**, S.R. Daly

INOR **344.** Low-symmetry subphthalocyanines as fluorescent probes and precursors for low symmetry phthalocyanines. **K. McAuliffe**, E.R. Trivedi

INOR **345.** Synthesis, characterization, and growth kinetics of LiOH and KOH synthesized surface modified zinc oxide quantum dots. A.D. Mena, D. Francis, **D. McCall-Butler**, **C. Walter**, J. Davis-Gun, S. Cabrera, A.T. Royappa, P.P. Vaughan, A. Schrock, K.S. Molek

INOR **346.** Withdrawn.

INOR **347.** Withdrawn.

INOR **348.** Synthesis, characterization, and growth kinetics of NaOH and CsOH-synthesized surface-modified Zinc oxide quantum dots. A.D. Mena, D. Francis, D. McCall-Butler, C. Walter, **J. Davis-Gunn**, **S. Cabrera**, A.T. Royappa, P.P. Vaughan, A. Schrock, K.S. Molek

INOR **349.** Synthesis and x-ray single crystal structure characterization of new platinum(II) complexes with O,N,N,O donor salen-type ligands. **G. Gonzalez Garcia**, Y. Saldaña González, J. López J., A. González García

INOR **350.** Isomerization in gold(I) compounds with 1,2-bis(diphenylphosphine) ethylene and fluorinated thiolates. **G. Romo**, G. Moreno-Alcantar, H. Torrens

INOR **351.** Withdrawn.

INOR **352.** Molybdenum(IV)oxophthalocyanines for Szilárd-Chalmers production of ^{99}Mo. V. Rosecker, P. Weinberger, **J.M. Welch**

INOR **353.** Study of multielectron redox chemistry through multiple bonded bimetallic asymmetric systems. **N. Rodriguez**, D. Portillo, D. Villagran

INOR **354.** Synthesis and characterization of molybdenum bimetallic complexes with non-symmetric formamidinate ligands. **I. Cervantes**, D. Villagran

INOR **355.** Diverse electronic structure of ruthenium coordinated in situ generated redox active 1,2-dinitrosobenzene and 2-nitrosoanilido. **P. Ghosh**, G.K. Lahiri

INOR **356.** Novel polycyclic thiones: Synthesis and complexation. **D. Tapu**, **R. Hooper**, **O. Kuykendall**

INOR **357.** Synthesis and titration studies of arylazothioformamide ligands with various metals towards quantifying material purification. **N.A. Johnson**, S.R. Wolfe, K.V. Waynant, J.G. Moberly, M.F. Roll

INOR **358.** Alterations of synthetic routes result in several new novel copper phenanthroline coordination complexes. **M. Wilk**, S. Scott, K. Reyes, V. Nesterov, M. Omary

INOR **359.** Magnetic exchange between ions of the first transition series in dimeric compounds using naphthazarin as bridging ligand. **E.N. Jimenez-Alvarado**, G. Valle-Bourrouet

INOR **360.** Synthesis and complexation of a new thione ligand. **P. Jean**, B. Hunt, D. Tapu

INOR **361.** Functionalized pyridylphosphine ligands: Synthesis and coordination chemistry with late transition metals. **M. Bezpalko**, W.S. Kassel

INOR **362.** Synthesis and characterization of heterobimetallic complexes supported by substituted trispyridylphosphines. **J. Leonard**, A.K. Frampton, W.S. Kassel

INOR **363.** Synthesis and characterization of saccharinate complexes of dirhodium. **S.C. Haefner**

INOR **364.** Synthesis and characterization of bimetallic ruthenium-platinum molecular cluster complexes with N-heterocyclic carbene complexes. **S. Etezadi**, B. Captain

INOR **365.** Formation of radical anions on the dipyrrin-1,9-dione scaffold of heme metabolites. **R. Gautam**, E. Tomat

INOR **366.** Singlet fission-based frameworks. **R. Hernandez Sanchez**, M. Trinh, D. Erdosy, X. Zhu, C.P. Nuckolls

INOR **367.** Synthesis and characterization of some dinitrosyl iron diphosphine compounds. **M.W. Jones**, V. Acquah, N. Jourabchian, N. Khojandi

INOR **368.** Addition reactions of some dinitrosyl iron diphosphine complexes. **R. Manandhar**, B. Alajmi, M.W. Jones

INOR **369.** Thiopyridazine based copper boratrane chemistry. **S. Holler**, M. Tüchler, F. Belaj, K. Kirchner, N. Mösch-Zanetti

Section H

Moscone Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Organometallic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

5:30 - 7:30

INOR **370.** Examination of the relative impact of tris(diisopropylphosphinomethyl)phenylborate and tris(diphenylphosphinomethyl)phenylborate in salts of $[M(CO)_3(PhBP_3)]^-$ (M = Cr, Mo, W). **S. Senthil**, J.T. Stephan, M.D. Storlie, M.L. Swift, V.G. Young, Jr., P.J. Fischer

INOR **371.** Bimetallic complexes of tris(diisopropylphosphinomethyl)phenylborate and tris(diphenylphosphinomethyl)phenylborate. **J.T. Stephan**, S. Senthil, M.D. Storlie, M.L. Swift, V.G. Young, Jr., P.J. Fischer

INOR **372.** Macrocyclic osmium carbonyl complexes with dicarboxylato ligands. **D.M. Marolf**, J.E. Johnstone, D.F. Zometa Paniagua, G.L. Powell

INOR **373.** Ligand development for iron catalyzed atom transfer radical polymerization. **M.R. Donley**, S.E. Jenny, T. Dudley, D.L. Zubris

INOR **374.** New Insights into the reactivity of tris(triphenylphosphine)ruthenium(II) dichloride. **M. Aristov**, K.B. Ghiassi, X.B. Powers, M.M. Olmstead, A.L. Balch

INOR **375.** Synthesis and reactivity of bis(NHC)borate titanium(IV) imido complexes. **M.G. Bernbeck**, J.A. Ziegler, R.G. Bergman, J. Arnold

INOR **376.** Synthesis and crystal structure of (dppe)PtH($SnPh_3$). **A. Schmiechen**, T.A. Mobley, I.A. Guzei

INOR **377.** Hydrogenation of carbon dioxide with ruthenium bis(pyridyl) isoindolene complexes. **J.L. Ciatti**, J.B. Geri, N.K. Szymczak

INOR **378.** Synthesis and reactivity of $Fe(TSPE)_2HCl$ for natural gas purification. **B. Han**, L.N. Zakharov, J.W. Gohdes

INOR **379.** Diiron carbonyl photochemical carbon monoxide releasing compound or PhotoCORM. C. Stephenson, E. Duran, **C.F. Works**

INOR **380.** Late transition metal compounds with 1,1′-bis(phosphino)ferrocene ligands. **N. Lauricella**, S. Hartlaub, C. Ryczek, A. Furneaux, J.D. Melton, N.A. Piro, W.S. Kassel, C. Nataro

INOR **381.** Substitution reactions of compounds containing 1,1′-bis(phosphino)ferrocene ligands. **N. Wamser**, K. Cabrera, C. Nataro

INOR **382.** Assessing CMPO-based ligands for selective lanthanide extraction from acidic solution. **M. Patterson**, O. Sode, S.M. Biros, E.J. Werner

INOR **383.** Synthesis and catalytic assessment of palladium complexes bearing bridging and pendant amine bis(phenolate) ligands. **E. Collins**, **B.J. Graziano**, B. Wile

INOR **384.** $B_{12}(OR)_{12}$ Reagents as tunable one-electron oxidants. **P. Chong**, M. Messina, J.C. Axtell, Y. Wang, B. Upton, B.M. Hunter, S. Khan, J.R. Winkler, H.B. Gray, A. Alexandrova, H.D. Maynard, A.M. Spokoyny

INOR **385.** Synthetic and analytical studies of a series of organic quinone ligands for catalytic purposes. **J.N. Herring**, W. Cross Lopez, S. Kruse, S.K. Hurst

INOR **386.** Dibenzo[a,j]xanthylium derivatives: Analytical studies and characterization. **W. Cross Lopez**, J.N. Herring, S. Kruse, S.K. Hurst

INOR **387.** Novel phosphorous-based ligands for precious metal catalysts. **S. Kruse**, J.N. Herring, W. Cross Lopez, S.K. Hurst

INOR **388.** Organophosphate alcoholysis by polymer-supported molybdenum peroxo complexes. **L. Miao**, L.Y. Kuo

INOR **389.** Computational investigation of phosphonothioate-neurotoxin hydrolysis by monomeric MoO_4^{2-}. **E. Bright**, L.Y. Kuo

INOR **390.** Catalytic and electrochemical properties of pyridine substituted imidazolium salts and the corresponding NHC-M complexes. **R.J. Swails**, S. Kariofillis, R. Cerbone, A. Conner, M. Sebold

INOR **391.** Synthesis of gold(III) complexes containing phenanthroline- or quinoline-based ligands. **K.M. Gilmore**, R.L. Marley, J.E. Thompson, G.R. Donalson, A.R. McCormick, C.P. Owens, S.R. Weller, I. Nizalowski, A.L. Rheingold, D.R. Weinberg

INOR **392.** Comparison of C-H bond cleavage in a series of palladium carboxylate complexes. **I.L. Hunter**, J. Jacobson, G.L. Bourne, A.N. Rainsberry, T. Kowalczyk, **M.L. Scheuermann**

INOR **393.** Synthesis and reactivity of molybdenum carbon dioxide complexes. **M.E. Graziani**, **X. Duan**, L.J. Briggs, G.R. Lorzing, J.R. Vasta, M.A. Pogash, P.M. Graham

Section I

Moscone Center
Hall D

Switchable Catalysts

J. A. Byers, P. Diaconescu, *Organizers*

5:30 - 7:30

INOR **394.** Redox switchable catalysts for the synthesis of block copolymers and crosslinked polymers. **K.R. Delle Chiaie**, A.B. Biernesser, J.A. Byers

INOR **395.** Application of bulk electrolysis methods to redox-switchable catalysis. **S. Quan**, J. Brosmer, P. Diaconescu

INOR **396.** Switchable di-zinc macrocycle catalysts: From highly active lactide polymerization to block copolymers. **A.A. Thevenon**, C. Romain, M. Bennington, H. Davidson, A. White, S. Brooker, C.K. Williams

INOR **397.** Redox switchable copolymerization of cyclic esters and epoxides by a zirconium complex. S. Quan, **R. Zhang**, P. Diaconescu

INOR **398.** Investigations into fast switching for the redox-switchable ring-opening polymerization of epoxides and lactides. **J.A. Kehl**, J. Curley, M. Qi, J.A. Byers

INOR **399.** DFT studies of redox switchable copolymerization of cyclic esters and epoxides. **J. Wei**, **P. Diaconescu**

INOR **400.** Ligand effect of a redox-controlled Al-based ROP catalyst. **A. Lai**, P. Diaconescu

INOR **401.** Yttrium and indium alkoxide complexes as redox switchable catalysts. **S. Ro**, A. Laughlin, P. Diaconescu

INOR **402.** Polymerization through redox switchable catalysis. **M. Riffel**, J. Wei, P. Diaconescu

INOR **403.** Redox switchable polymerization reactions. **R. Dai**, P. Diaconescu

INOR **404.** Progress towards parameterizing flow reactor design for the efficient scale-up of photoredox catalysis methods. **T.M. Williams**, A. Sun, C. Stephenson

INOR **405.** Ferrocene-Chelating heteroscorpionate complexes in catalysis. **M. Abubekerov**, P. Diaconescu

INOR **406.** Hydroamination through redox-switchable catalysis. **Y. Shen**, S.M. Shepard, P. Diaconescu

Section J

Moscone Center
Hall D

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of John E. Bercaw

A. Hazari, N. Hazari, *Organizers*

5:30 - 7:30

INOR **407.** Understanding the mechanism of catalytically upgrading (bio)ethanol to butanol. **H. Aitchison**, D. Wass, R. Wingad

Section K

Moscone Center
Hall D

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

5:30 - 7:30

INOR **408.** Single chain polyethylene nanocrystals. **M. Schnitte**, A. Godin, P. Kenyon, M. Krumova, I. Goettker Genannt, S. Mecking

INOR **409.** Copolymerization of cyclohexene oxide with carbon dioxide catalyzed by dinuclear iron complex bearing a phenylene-bridged bis(tripodal N_2O_2) ligand. **S. Zhan**, Q. Jiang, Z. Song

INOR **410.** Ethylene insertion polymerization in the presence of organic radicals - Exploiting mechanistic insights to influence microstructures. **S. Stadler**, F. Ölscher, I. Göttker-Schnetmann, V. Monteil, S. Mecking

INOR **411.** Model studies of catalytic olefin chain growth in the presence of biological impurities. **F.P. Wimmer**, I. Göttker-Schnetmann, S. Mecking

INOR **412.** Remote substituent effects in Ni(II)-catalyzed chain growth catalysis. **E. Schiebel**, T. Wiedemann, I. Goettker Genannt, S. Mecking

INOR **413.** Catalytic upgrading of fatty acids from renewable single cell oils. **J. Zimmerer**, L. Williams, D. Pingen, S. Mecking

INOR **414.** Development of coordinatively unsaturated, low-valent metal isocyanide MOFs. **A. Arroyave**, D. Agnew, J.S. Figueroa

INOR **415.** Withdrawn.

Section L

Moscone Center
Hall D

Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

5:30 - 7:30

INOR **416.** Synthesis and characterization of organometallic compounds of coinage metals relevant to catalysis. **S. Martínez de Salinas Uzquiza**, Á. Mudarra, M. Pérez-Temprano

INOR **417.** Mechanistic studies on the oxidative addition of aryl halides to COBALT(I) complexes. **M. Perez-Temprano**, J. San Jose, D. Gallego

INOR **418.** Precision measurement of the C(sp^3)-H activation kinetic isotope effect in a ruthenium-centered olefin metathesis catalyst via differential ^{13}C labeling. **C. Galvin**, A. Johns, R.L. Pederson, J. Cannon, R.H. Grubbs, D.J. O'Leary

INOR **419.** N-Heterocyclic Olefins (NHO) as ancillary ligands in catalysis and their application in transfer hydrogenation reactions. **J. E A**, M. Iglesias, N. Garcia Villalta, L.A. Oro

INOR **420.** Iridium(III) bis-*N*-heterocyclic carbenes catalysed transfer hydrogenation reactions. **N. Garcia Villalta**, L.A. Oro, M. Iglesias, J. E A

INOR **421.** Synthesis and reactivity of the aminovinyl carbenes toward alkynes in the Dötz reaction. **R.M. Padilla**, **J. Tamariz**, **F. Delgado**, **A. Feliciano**

INOR **422.** Reactivity of biaryl mono-phosphine complexes. **B.E. Silva**, K. Sukert, H. Henriksen, D.B. Grotjahn

Section M

Moscone Center
Hall D

Undergraduate Research at the Frontiers of Inorganic Chemistry

Solid State & Materials Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

5:30 - 7:30

INOR **423.** Synthesis and characterization of metal-organic framework materials for aqueous heavy metal detection. N.S. Morey, **T.E. Bustamante**

INOR **424.** Singlet fission in a hybrid system with CdSe nanocrystals and functionalized chromophores. **D.S. Hamilton**, X. Li, M.L. Tang

INOR **425.** Design of Polyethylene Glycol (PEG)-grafted gold nanoparticles for biomedical applications. **J. Grundler**, T. Lafferty, **E. Park**

INOR **426.** Effects of seasonal variation of groundwater composition on gold nanoparticle surface chemistry. **E.R. Carlson**, A.K. Bentley

INOR **427.** Catalytic activity of ultrasmall copper nanoparticles. **A. Kale**, G. Ferko, S.K. St Angelo

INOR **428.** Dye encapsulation in metal-organic frameworks. **B.J. Johnson**, K. Anderson, E. Goyke, K. O'Connor, N. Anderson, N. Beaulieu

INOR **429.** Single step synthesis of Sb/Cu-doped ZnO and ZnS nanostructures on mica and n-GaN/Al_2O_3 substrates by a simple vapor phase transport method. **H. Rivera-Marrero**, T.M. Trad, M.J. Uddin

INOR **430.** Withdrawn.

INOR **431.** Electrochemical characterization of manganese dioxide supercapacitors. **B.T. Hohman**, R.S. Zickel, A.K. Bentley

INOR **432.** Fabrication of hierarchical nanostructures for surface-enhanced Raman scattering biosensors. **K. Curtin**, N. Wu

INOR **433.** Understanding secondary structures of metal organic frameworks via tuning of ligand-ligand interactions. M. Johnson, M.J. Voegtle, **K. Tran**, J. Jones, C. Bauer

INOR **434.** Growth of microporous imidazolate frameworks in mild conditions via polymer-templating. **C. Bauer**, K. Kwong, B. Doyle, H. Kim

INOR **435.** Negative fingerprints development on reducing metal substrates. **N. Zuparova**, L. Mullen, L. Bliss, A. Lafi, H. Abdou, A. Mohamed

INOR **436.** Gold nanoparticle catalysts: Chemical properties and catalytic behavior. **M.N. Pollock**, **C. Peterson**, C. Pursell, B.D. Chandler

INOR **437.** Varying zinc sulfide nanocrystal shape, size, and surface chemistry to control copper doping via cation exchange. **H.M. Sizemore**, K.N. Heupel, J.L. Jenkins

INOR **438.** Ligand effects on the reactivity and synthesis of bimetallic molecular precursors for semiconductor materials. **J.L. Tennant**, L.J. Maxton, A.W. Holland

INOR **439.** Hydrogenation over metal oxide supported gold nanocatalysts. **A. Huther**, H. Krause, C. Pursell, B.D. Chandler

INOR **440.** Understanding growth behavior of alumina (Al_2O_3) and boehmite (AlO(OH)) nanoparticles. **M. Casillas**, F.A. Fasulo, N.S. Bell, T.J. Boyle, L.J. Treadwell, B.A. Hernandez-Sanchez

Section N

Moscone Center
Hall D

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Materials Chemistry of Solutions & Solids for a Sustainable Future

J. C. Giordan, S. E. Hayes, B. L. Maddux, *Organizers*

5:30 - 7:30

INOR **441.** Film formation from peroxo hexatantalate precursors. **R.H. Mansergh**, L.B. Fullmer, D. Park, J.M. Amador, M.D. Nyman, D.A. Keszler

INOR **442.** Enhanced dehydroxylation and interface passivation of solution-processed dielectric metal oxide thin films using forming gas annealing. **J.C. Ramos**, F. Luo, B.A. Hammann, D. Park, Y. Huang, S.E. Hayes, E.L. Garfunkel, D.A. Keszler

INOR **443.** Amorphous niobium phosphate thin films from clusters in water. **D. Park**, S. Goberna-Ferron, D. Fast, M. Dolgos, M.D. Nyman, D.A. Keszler

INOR **444.** Aqueous solution-derived lanthanum zirconium oxide thin films on Self-Assembled Monolayers (SAMs). **M.C. Thomas**, K.N. Woods, C. Page, Y.J. Chabal

INOR **445.** Solution-processed low-refractive index alumina-based thin films for anti-reflective coatings. **C.K. Perkins**, M.T. Gutierrrez-Higgins, V. Goulioukk, R. Mansergh, D. Park, J.C. Ramos, C. Nanayakkara, Y.J. Chabal, D.A. Keszler

INOR **446.** Improved synthesis of the elusive aluminum hydroxide octamer $[Al_8(OH)_{14}(H_2O)_{18}]^{10+}$ cluster. **E. Eitrheim**, **C.K. Perkins**, L.B. Fullmer, B. Fulton, C. Colla, A.F. Oliveri, D. Park, W.H. Casey, M.D. Nyman, T. Forbes, D.W. Johnson, D.A. Keszler

INOR **447.** Understanding the effect of counterions on the hydrolysis of aqueous aluminum hydroxo clusters using QM computations. **L. Wills**, J. Buchanan, C.K. Perkins, B. Fulton, D.A. Keszler, D.W. Johnson, P. Cheong

INOR **448.** Reactions of hexatantalate and hexaniobate with hydrogen peroxide. **C.E. Malmberg**, L. Wills, L.B. Fullmer, M.D. Nyman, P. Cheong

INOR **449.** Proton-exchange rates on hydroxide bridges of mineral-like metal hydroxide clusters. **C.R. Fields**, A. Oliveri, C. Colla, W.H. Casey, D.W. Johnson

INOR **450.** Solution speciation of amphoteric early transition metal clusters. **D. Hutchison**, M. Olsen, M.D. Nyman

INOR **451.** Tin and alkyltin speciation on aqueous and nonaqueous solutions. **M. Olsen**, D. Hutchison, S. Saha, M.D. Nyman, D.A. Keszler

INOR **452.** Characterization of *n*-butyl-SnOOH for nanopatterning: Radiation behavior. **N. Kenane**, D.A. Keszler

INOR **453.** Characterization of *n*-butyl-SnOOH for nanopatterning: Solution precursor and film. **J.M. Amador**, J.T. Diulus, M. Li, R.T. Frederick, S. Saha, E.L. Garfunkel, D.A. Keszler, G.S. Herman

INOR **454.** Characterization of n-BuSnOOH: Solution precursor identity and film quality. **M. Li**, J.M. Amador, R.T. Frederick, S. Saha, J.T. Diulus, D.A. Keszler, G.S. Herman, E.L. Garfunkel

INOR **455.** Characterization of butyl tin photoresists with electron stimulated desorption and temperature programmed desorption. **R.T. Frederick**, J.T. Diulus, S. Saha, J.M. Amador, M. Li, D.A. Keszler, E.L. Garfunkel, G.S. Herman

INOR **456.** Withdrawn.

INOR **457.** Glass formation in basic halogenides of zirconium and hafnium. **J.A. Sommers**, J.M. Amador, E.C. Fong, D.A. Keszler

INOR **458.** Light emission from an electrical conductor. **V. Goulioukk**, K.A. Stewart, R.G. Manley, D.G. Enicks, J.F. Wager, D.A. Keszler

INOR **459.** Design meets nature: New tetrahedrite superabsorbers. **J. Heo**, D.A. Keszler

INOR **460.** Photochemical reaction coordinates of metal-organic complexes in solution revealed by femtosecond electronic and Raman spectroscopy. **L. Zhu**, S. Saha, Y. Wang, N.D. Rozanov, D.A. Keszler, C. Fang

INOR **461.** Effects of Organic Components on Novel Hybrid Organic-Inorganic Structures. **B. Barraza**, R. Seshadri

‡ *Cooperative Cosponsorship*

Section O

Moscone Center
Hall D

Sustainability in Electrocatalytic Fuel & Chemical Production

Cosponsored by CATL

L. A. Berben, J. L. Dempsey, *Organizers*

5:30 - 7:30

INOR **462.** Silicon-based photoelectrochemical cell for enzymatic CO_2 conversion. **J. Ko**, E. Son, S. Kuk, C. Park

INOR **463.** Towards formic acid oxidation by surface attached $Ni(P_2N_2)_2$ complexes. **F. Brunner**, C.P. Kubiak

Section P

Moscone Center
Hall D

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

Cosponsored by WCC

X. Bu, P. Yang, Q. Zhang, D. Zhao, N. Zheng, *Organizers*

5:30 - 7:30

INOR **464.** Constrained Volume self-assembly of organic–inorganic nanocomposites. **R. Liu**

INOR **465.** Facile synthesis of nanosheet AuPd/g-C_3N_4 composites for photocatalytic H_2 evolution under visible-light irradiation. **L. Ge**, C. Han

INOR **466.** Photochemical method in preparing atomically dispersed catalysts. **P. Liu**, Y. Zhao, G. Fu, N. Zheng

INOR **467.** Design of (metallo)porphyrin-based coordination frameworks for electrochemical studies. **Q. Lin**

INOR **468.** Dichalcogenide ligand exchange on germanium nanoparticles. **K.A. Newton**, A.L. Holmes, S. Kauzlarich, W. Blacklock

INOR **469.** Aromatic guest molecules mediated synthesis of porous homochiral camphorate frameworkds. **J. Jin**, X. Zhao, X. Bu

INOR **470.** Nanoporous carbon derived from a functionalized metal–organic framework as highly efficient oxygen reduction electrocatalyst. **Y. Wang**, P. Feng

INOR **471.** Applications of heterometallic MOFs in gas adsorption, separation and biodiesel preparation. **Y. Wang**, Q. Zhai, P. Feng

INOR **472.** Chirality in atomically precise noble nanoclusters. **J. Yan**, B.K. Teo, N. Zheng

INOR **473.** Multivariable modular design of pore space partition. **X. Zhao**, E.T. Nguyen, X. Bu, P. Feng

INOR **474.** Rational tuning of structure type in open framework chalcogenide. **X. Chen**, X. Bu, P. Feng

INOR **475.** Crystallography in MOF: Ordering guest molecules by coordination assisted orientation control. **L. Wang**, S. Cohen

INOR **476.** Electrochemiluminescence behaviors featuring the point defects of supertetrahedral chalcogenide nanocluster. **Y. Liu**

INOR **477.** Metal-free peralkylation of the *closo*-hexaborate dianion, $B_6H_6^{2-}$. **J. Axtell**

INOR **478.** Synthetic design of homochiral metal-organic frameworks. **E.T. Nguyen**, X. Zhao, X. Bu

INOR **479.** Novel metal organic frameworks through tetrameric magnesium clusters. **A. Hong**, X. Zhao, A. Hong, X. Bu

Section Q

Moscone Center
Hall D

Nanoscience

B. G. Trewyn, *Organizer*

5:30 - 7:30

INOR **480.** Synthesis, characterization, and application of dendrimer coated silica nanoparticles as fluorescent chemosensors. **H. Deuermeyer**, A. Luhrs, L.D. Margerum

INOR **481.** Ag-TiO_2 hybrid nanoparticles as active photocatalyst for hydrogen evolution. **S. Varapragasam**, S. Mia, C. Balasanthiran, R.M. Rioux, J.D. Hoefelmeyer

INOR **482.** Gold nanorods with a photoresponsive azobenzene shell via *in-situ* reduction of 4-nitrobenzenediazonium tetrafluoroborate. **D.H. Wang**, K. Park, R.A. Vaia, L. Tan

INOR **483.** Lead chalcogenide quantum dots: Measurements on a standardized sample. **A. Marshall**, J.C. Johnson, J. Luther, A.F. Fidler, V.I. Klimov, M.C. Beard

INOR **484.** Advantages of naked Ru^0 surfaces in catalysis and electrocatalysis. S. Anantharaj, **S. Kundu**

INOR **485.** Toward large-area Surface Enhanced Raman Spectroscopy (SERS) sensors: Fabrication of patterned, nanostructured surfaces. **W. Mihalyi-Koch**, **A. Shadrav,** A. Oh, F. Dawood

INOR **486.** Fabrication of highly nanostructured electrodes. **P. Kharel**, A. Talsania, D. Cahill, F. Dawood

INOR **487.** Carbon-based nanomaterials applications in the photo-triggered release of small molecule bioregulators. **P. Huang**, X. Zhao, X. Dang, N. Zheng, P.C. Ford

INOR **488.** Fundamental differences in the cation exchange behaviors of cadmium- and lead chalcogenide quantum dots. **X.A. Aguilar**, C. Lin, A.L. Morris, S.E. Benjamin, P.G. Van Patten

INOR **489.** Nanotethering to cadmium selenide for solar applications. **D. Jackson**, M.E. Hagerman, J.D. Kehlbeck

INOR **490.** Studying the surface effects of PEDOT:PSS on nanoporous $LiMn_2O_4$. **V. Basile**, B. Lesel, S.H. Tolbert

Deposition & Etching of Nanostructures

Posters

Sponsored by COLL, Cosponsored by INOR

MONDAY MORNING

Section A

Moscone Center
Gateway Ballroom 103/104

ACS Awards in Inorganic Chemistry: Plenary Session

S. A. Koch, N. S. Radu, *Organizers*

J. D. Protasiewicz, *Organizer, Presiding*

8:15 INOR **491. Award Address** (ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry sponsored by Strem Chemicals, Inc.). Copper-Oxygen complexes relevant to enzyme intermediates. **W.B. Tolman**

8:50 INOR **492. Award Address** (Harry Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator sponsored by the Gray Award Endowment). Rational development of pincer supported iron complexes for the reversible hydrogenation of carbon dioxide to formic acid and methanol. **N. Hazari**, W.H. Bernskoetter

9:20 INOR **493. Award Address** (ACS Award in Inorganic Chemistry sponsored by Aldrich Chemical Company, LLC). Amazing nonheme high-valent iron-oxo landscape. **L. Que**

9:55 Intermission.

10:10 INOR **494. Award Address** (ACS Award in Organometallic Chemistry sponsored by The Dow Chemical Company Foundation). Hydrogenase- and ACS-inspired bioorganometallic chemistry. **M.Y. Darensbourg**

10:40 INOR **495. Award Address** (F. Albert Cotton Award in Synthetic Inorganic Chemistry sponsored by the F. Albert Cotton Endowment Fund). Crystalline semiconducting and porous materials: Synthesis, properties, and applications. **P. Feng**

11:10 INOR **496. Award Address** (Gabor A. Somorjai Award for Creative Research in Catalysis sponsored by the Gabor A. & Judith K. Somorjai Endowment Fund). Mechanistic studies of 1-alkene trimerization and polymerization with organo-transition metal catalysts. **J.E. Bercaw**

11:40 INOR **497. Award Address** (ACS Award in the Chemistry of Materials sponsored by E. I. du Pont de Nemours & Co.). Inorganic materials chemistry and innovation. **D.A. Keszler**

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Sponsored by PHYS, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

MONDAY AFTERNOON

Section A

Moscone Center
2009

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of John E. Bercaw

A. Hazari, *Organizer*

N. Hazari, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR **498.** Stoichiometric and catalytic reactions mediated by water-soluble host-guest supramolecular systems. **R.G. Bergman**

2:00 INOR **499.** Organometallic chemist's nightmare: Chemistry in air, water, and heterogeneous environments. **L. Do**, A. Ngo, S. Bose, L. Yang

2:25 INOR **500.** Polymerization catalysts that benefit from dynamic ligand behavior. **J.A. Byers**, N.K. Szymczak, J.A. Kehl, A. Kaur, C.M. Manna, K.T. Tseng, L.V. Hale, A.B. Biernesser

2:50 INOR **501.** Biologically inspired clusters: Synthetic control of structure and effects on reactivity. **T. Agapie**

3:15 Intermission.

3:25 INOR **502.** Metal oxo cubanes as catalytic centers for oxygen evolution. **T.D. Tilley**, A. Nguyen

3:50 INOR **503.** Versatile redox chemistry of nanoscale cerium oxide. **J.M. Mayer**, D. Damatov, S. Laga, J. Peng

4:15 INOR **504.** One and two dimensional cobalt dithiolene frameworks for artificial photosynthesis. **S.C. Marinescu**, A.J. Clough, C.A. Downes

4:40 INOR **505.** From single atom based-catalysts to nanoparticles. **E. Bunel**

5:05 INOR **506.** Recent advances in olefin metathesis. **R.H. Grubbs**

Section B

Moscone Center
2011

Celebrating 60 Years of the Division of Inorganic Chemistry

Former Young Investigators

M. J. Clarke, D. C. Crans, *Organizers*

J. R. Long, J. D. Protasiewicz, N. Radu, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **507.** Multi-electron redox chemistry: Redox load distributions in cluster cores. **T. Betley**

2:05 INOR **508.** Metals and immunity: Explorations of a biological hexahistidine site. **E.M. Nolan**

2:35 INOR **509.** Plasmon enhanced solar steam generation and desalination. **J. Zhu**

3:05 INOR **510.** Single-molecule magnets based on oligo- and polynuclear lanthanide complexes. E. Mazarakioti, J. Tang, G. Christou, **T. Stamatatos**

3:35 Intermission.

3:50 INOR **511.** Filled tetrahedral semiconductors: Solution phase synthesis of low dimensional intermetallics. **J. Vela-Becerra**

4:20 INOR **512.** Graphite-Conjugated catalysis. **Y. Surendranath**

4:50 INOR **513.** Synthesis, characterization, and reactivity of redox active 2,5-diiminopyrrole ligands and complexes. **J.S. Anderson**, A.J. McNeece

5:20 INOR **514.** Responsive chemical tools for COS and H_2S delivery. **M.D. Pluth**

Section C

Moscone Center

2016

Undergraduate Research at the Frontiers of Inorganic Chemistry

Solid State & Materials Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

S. Poland, *Presiding*

1:30 INOR **515.** Synthesis and properties of transition metal carbide buckypaper. **K.E. Madsen**, B.M. Leonard

1:50 INOR **516.** Super robust and water-soluble gold nanoparticles for biomedicine. **L. Mullen**, L. Bliss, N. Zuparova, B. Atallah, H. Abdou, A. Mohamed

2:10 INOR **517.** Using carboxylate ligand sterics to control copper availability during cation exchange to yield Cu-doped ZnS nanocrystals. **K.N. Heupel**, H.M. Sizemore, J.L. Jenkins

2:30 INOR **518.** Characterization of silver (I) and engineered Silver Nanoparticle (AgNP) binding to apo and metal reconstituted zinc finger peptides. **Z. Amaris**, G.A. Park, M. Eiken, K.E. Splan, K. Wheeler

2:50 Intermission.

3:05 INOR **519.** Coordination compounds and hybrid materials containing the hydrtris(3,5-dimethyl-1,2,4-triazolyl)borate ligand. E.T. Roberts, K.L. Salvatore, B.C. Chan, **B.A. Reisner**

3:25 INOR **520.** Synthesis of UO_2-Zircaloy thin films to address pellet-cladding debonding. **B. Klamm**, R.F. Hess, T.J. Boyle, K. Hattar, R. Dingreville, D. Perales

3:45 INOR **521.** Advances in manganese- and cobalt-based nanostructures for oxygen/hydrogen electrocatalysis. **J.A. Vigil**, T.N. Lambert

4:05 INOR **522.** Understanding titanium and sulfur speciation in titanium trisulfide electrodes using x-ray spectroscopy. **C. Wilson**, V. Doan-Nguyen, J.D. Bocarsly, A. Lanzirotti, R. Seshadri

4:25 INOR **523.** Synthesis of quantum dot bioimaging agents to study bacteriophage. **S. Mendoza**, M. McKeown, M. Casillas, C. Stevens, J. Pelowitz, A. McBride, C. Ashley, B.A. Hernandez-Sanchez

Section D

Moscone Center

2018

ACS Awards: Symposium in honor of Lawrence Que, Jr. & William B. Tolman

P. L. Holland, M. J. Maroney, *Organizers*, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **524.** Bioinorganic aspects of nitrogen oxide chemistry with heme and/or copper complexes. **K.D. Karlin**

2:00 INOR **525.** Synthetic chemistry as a window into biology: Architectural complexity at the molecular level. **A. Borovik**

2:25 INOR **526.** Cleaving and forming C–H bonds by moving protons and electrons. **J.M. Mayer**, J. Darcy, T. Markle, S. Kolmar

2:50 INOR **527.** Oxygen activation and C-H bond cleavage by metalloenzymes and metalloporphyrins. **J.T. Groves**

3:15 Intermission.

3:30 INOR **528.** Bioinorganic spectroscopy: Activating metal sites for biological electron transfer. **E.I. Solomon**

3:55 INOR **529.** Insights into the electronic structure of iron sulfur clusters using two-dimensional x-ray spectroscopy. **S. DeBeer**

4:20 INOR **530.** Bio-inspired bimetallic complexes for activating H_2 and CO_2. **C. Lu**, R. Cammarota, S. Desai, J. Xie, K. Vogiatzis, D. Pahls, L. Gagliardi

4:45 INOR **531.** Tracking mobile zinc in the brain - new probes, new biology. **S.J. Lippard**

Section E

Moscone Center

2020

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

K. R. Kittilstved, *Organizer*

E. J. McLaurin, *Organizer, Presiding*

A. Greytak, *Presiding*

1:30 INOR **532.** Chemically tunable 2D layered materials. **K.J. Koski**

2:00 INOR **533.** Solution-Phase approaches to indium nitride nanomaterials: Chemical insights on a new mechanism. Y. Chen, Z. Liu, N.S. Karan, **R. Beaulac**

2:30 INOR **534.** Linking the forward and reverse vapor-liquid-solid mechanisms in metal oxide nanostructures. L. Yu, B.M. Hudak, A.J. Riddle, S. Wang, Y. Chang, **B. Guiton**

3:00 Intermission.

3:15 INOR **535.** Patterns and plasmonics: Nanopatterning of silicon surfaces via directed self-assembly. F. Liu, E. Luber, B. Olsen, **J.M. Buriak**

3:45 INOR **536.** Responsive and reconfigurable materials from dimensionally confined colloidal nanocrystal assemblies. **B. Helms**, Z. Zhang, E. Goldfine, C. Huang, T. Russell

4:15 INOR **537.** Nanomaterial surfaces in 0, 1, and 2 dimensions: Results from chromatography and functional imaging. **A.B. Greytak**

Section F

Moscone Center

2022

Sustainability in Electrocatalytic Fuel & Chemical Production

Cosponsored by CATL

L. A. Berben, J. L. Dempsey, *Organizers*

C. A. Caputo, *Presiding*

1:30 INOR **538.** Sustainable solar-to-fuels and solar-to-fertilizer production. **D.G. Nocera**

1:55 INOR **539.** Reducing overpotential and maintaining high rates in nickel electrocatalysts for H_2 production. **M.J. O'Hagan**, A.P. Cardenas, A.M. Appel, R. Bullock, E.S. Wiedner

2:20 INOR **540.** Unravelling PCET pathways of the hydride formation step in cobalt complexes relevant to solar fuel production. **N. Elgrishi**

2:40 INOR **541.** Electrocatalytic reduction of CO_2 using cyclopentadienone iron complexes. **R. Francke**, A. Rosas-Hernandéz, H. Junge, M. Beller, M. Roemelt

3:05 INOR **542.** Earth-abundant metal complexes with flexible ligand coordination for catalytic proton and carbon dioxide reduction. S. Saund, K. Ng, S. Goldschmid, **V. Thoi**

3:30 Intermission.

3:45 INOR **543.** Variable temperature spectral and electrochemical studies of carbon dioxide redcution by [Fe4N(CO)12]-: Mechanistic investigations. **A. Taheri**, L.A. Berben

4:05 INOR **544.** Bioinorganic approaches to solar-to-chemical conversion: Merging molecular catalysis with materials and biology. **C.J. Chang**

4:30 INOR **545.** Catalytic production of hydroben and reduction of carbon dioxide by dirhodium(II,II) complexes. **C. Turro**, K.R. Dunbar

4:55 INOR **546.** Homogeneous water oxidation and CO_2 reduction: Catalysts and mechanisms. Y. Xie, D.W. Shaffer, D. Szalda, **J.J. Concepcion**

Section G

Moscone Center

2024

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

P. Yang, Q. Zhang, D. Zhao, N. Zheng, *Organizers*

X. Bu, *Organizer, Presiding*

1:30 INOR **547.** Mo-S Complexes based on [MoO(S2)2] motif as MoS_x-inspired electrocatalysts for hydrogen production. **Y. Wu**, B. Garrett

1:50 INOR **548.** Compositional, structural, and geometrical design of crystalline porous materials. **X. Bu**

2:10 INOR **549.** Controlled encapsulation of catalysts into metal-organic frameworks. **C. Tsung**

2:30 INOR **550.** Controlling the structures and properties of gold/silver nanoclusters with unconventional protecting ligands. **Q. Wang**

2:50 INOR **551.** Surfactant-thermal method to prepare crystalline inorganic materials. **Q. Zhang**

3:10 Intermission.

3:40 INOR **552.** Crystal engineering of titanium-oxo clusters. **J. Zhang**

4:00 INOR **553.** Stabilization of isolated metal chalcogenide nanoclusters and their electrocatalytic applications for hydrogen evolution reaction and oxygen reduction reaction. **T. Wu**

4:20 INOR **554.** Beyond multimetallic nanoparticles for catalysis: A general approach to stable high-index faceted multimetallic nanowires. **X. Huang**

4:40 INOR **555.** Metal nanoclusters as a model system for investigating the surface structure and catalysis of metal nanoparticles. J. Yan, L. Ren, P. Yuan, L. Huang, **N. Zheng**

Section H

Moscone Center

3000

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

A. Dudnik, *Presiding*

1:30 INOR **556.** Chiral Phospha[*n*] ferrocenophanes: New metallopolymers through ring-opening polymerizations. **M. Cao**, S. Sadeh, J. Quail, J. Müller

1:50 INOR **557.** Asymmetric hybrid salen/phosphasalen initiators for the iso-selective ring-opening polymerisation of rac-lactide. **C. Coleman**, C.K. Williams, N.J. Long

2:10 INOR **558.** Redox control of aluminum ring-opening polymerization: A combined experimental and DFT investigation. **J. Wei**, **P. Diaconescu**

2:30 INOR **559.** Synthesis of (salfen) In(OPh)$(OtBu)_2$ catalyst, and redox-swiychable ring-opening polymerization of e-caprolactone and other cyclic esters. S. Quan, **R. Zhang**, P. Diaconescu

2:50 INOR **560.** Highly robust Pd(II) α–diimine catalysts for olefin (co) polymerization. **S. Dai**, C. Chen

3:10 INOR **561.** Redox-controlled olefin (Co)polymerization catalyzed by ferrocene-bridged phosphine-sulfonate palladium complexes. **M. Chen**, C. Chen

3:30 INOR **562.** Supported lanthanide catalysts: Role of the grafting on the stereochemical outcome of different polymerization reactions. **I. Del Rosal**, L. Maron

3:50 INOR **563.** Investigation of a unique mechanism for the production of high molecular weight polyethylene using bis(pyridylimino)isoindolate iron(II) catalysts. **J.A. Kehl**, K.T. Tseng, L.V. Hale, A.B. Biernesser, N.K. Szymczak, J.A. Byers

4:10 INOR **564.** Mechanistic studies of Pd(II)-catalyzed copolymerization of ethylene and vinylalkoxysilanes: Evidence for a β-silyl elimination chain transfer mechanism. **Z. Chen**, W. Liu, O. Daugulis, M. Brookhart

4:30 INOR **565.** Non-chiral lithium aluminate reagents for the determination of enantiomeric excess of chiral alcohols. **R. Garcia**, D. Wright

4:50 INOR **566.** Withdrawn.

5:10 INOR **567.** Aqueous polyethylene nanocrystal dispersions from catalytic polymerization. **P. Kenyon**, A. Godin, S. Mecking

‡ *Cooperative Cosponsorship*

Section I

Moscone Center

3010

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Supported Organometallics & Heterogeneous Catalysis

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREM, Argonne National Lab, Northwestern University

A. Facchetti, T. Lohr, *Organizers*

M. Neurock, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **568.** Tuning nanoparticle alloys to enhance C-H bond activation for the catalytic dehydrogenation of ethane. V. Cybulskis, J.R. Gallagher, H. Tsent, B. Bukowski, Z. Wu, E.C. Wegener, A.J. Kropf, B. Ravel, J.P. Greeley, F. Ribeiro, **J. Miller**

2:05 INOR **569.** Hydrogen and formaldehyde generation from bio-derived alcohols using supported molybdenum-oxo catalysts. **T. Lohr**, A. Mouat, M. Delferro, P.C. Stair, T.J. Marks

2:35 INOR **570.** Integration of the three fields of catalysis: Heterogeneous, homogeneous, and enzyme. **G.A. Somorjai**

3:05 INOR **571.** Catalysts synthesized by organometallic surface chemistry. **P.C. Stair**

3:35 Intermission.

3:45 INOR **572.** Surface structural-chemical characterization of supported single-site organometallic catalysts. **M. Delferro**

4:15 INOR **573.** Metallacyclobutane structure influence on the production of propylene via olefin metathesis over surface organometallic chemistry derived catalysts. **C.P. Nicholas**, M. Taoufik

4:45 INOR **574.** Metal-organic Frameworks for Sustainable Catalysis. **W. Lin**

Section J

Moscone Center

3012

ACS Award in Organometallic Chemistry: Symposium in honor of Marcetta Y. Darensbourg

D. Mason, C. G. Riordan, *Organizers*

M. R. Mackiewicz, X. Zhao, *Presiding*

1:30 INOR **575.** Carbene-stabilization of elusive main group oxides. **G.H. Robinson**

1:55 INOR **576.** On the contents of metal-seamed metal organic nanocapsules. **J.L. Atwood**, C. Zheng, A. Rathnayake, R. Patil, K. Sikligar, K. Feaster, C. Barnes, P. Atwood, D.A. Atwood

2:20 INOR **577.** Exploiting the non-innocence of antimony ligands in organometallic catalysis. **F.P. Gabbai**

2:45 INOR **578.** Dinitrosyl Iron Complexes (DNICs): Synthesis and spectroscopic characterization toward unveiling the catalytic roles of DNICs. **W. Liaw**

3:10 INOR **579.** Platinum reagents modified for click chemistry: Towards high-throughput analysis of platinum drug targets. A.D. Moghaddam, K. Plakos, J.D. White, R. Cunningham, E. Reister, E. Sutton, M.M. Haley, **V. DeRose**

3:35 Intermission.

3:50 INOR **580.** C–H activation by a discrete superoxonickel complex. **C.G. Riordan**

4:15 INOR **581.** Pyridol derived N-heterocyclic amines and applications in coordination chemistry, catalysis, and medicine. **K.N. Green**, S.M. Brewer, H.M. Johnston, M.E. Burnett

4:40 INOR **582.** Fun with devil's copper and the odd oxidations of sulfur. **P.J. Farmer**, M. Kumar

5:05 INOR **583.** Hydrogenase/epoxide–CO_2 catalysis: Killing two birds with one cat. **D.J. Darensbourg**

Section K

Moscone Center

3001

Switchable Catalysts

P. Diaconescu, *Organizer*

J. A. Byers, *Organizer, Presiding*

B. P. Fors, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **584.** Regulating polymer stereomicrostructures and polymerization activity and chemoselectivity by ion pairs and Lewis pairs. **E.Y. Chen**

2:05 INOR **585.** Externally controlled chemistry: New methods for modulating polymerization and other transformations. **C. Bielawski**

2:35 INOR **586.** Potential applications of switchable catalysts for sustainable energy and water production. **M.A. Reynolds**

3:05 Intermission.

3:20 INOR **587.** Photocontrolled Cationic Polymerizations. **B.P. Fors**

3:50 INOR **588.** Switchable polymerization catalysts: Selective block copolymers from monomer mixtures. **C.K. Williams**

4:20 INOR **589.** Redox switchable catalysis applied to ring opening polymerization. **P. Diaconescu**

4:50 INOR **590.** Mechanistic trends from computational chemistry for the design of redox switchable catalysts. **T. Cantat**

Section L

Moscone Center

3003

Organometallic Chemistry: Synthesis & Characterization-Early Transition Metals

N. S. Radu, *Organizer*

T. K. Hollis, *Presiding*

1:30 INOR **591.** Extreme π-loading as a design element for accessing imido reactivity: CCC-NHC Ta bis(imido) pincer complex synthesis and reactivity in oxidative amination. T.R. Helgert, J.A. Denny, G.M. Lang, G. Liang, C.E. Webster, **T.K. Hollis**

1:50 INOR **592.** Diphenylacetylene reduction mediated by rare-earth naphthalene complexes supported by a ferrocene diamide ligand. **J.L. Brosmer**, W. Huang, P. Diaconescu

2:10 INOR **593.** Ring-opening reactions of quinoline and isoquinoline with a low-valent titanium alkyl complex. **T. Kurogi**, M. Baik, D.J. Mindiola

2:30 INOR **594.** Probing the stability & reactivity of early first-row transition metal centers in low-coordinate environments supported by silylaryl-amido ligands. **I.C. Cai**, T.D. Tilley

2:50 INOR **595.** Oxidative group transfer reactions on macrocyclic N-heterocyclic tetracarbene chromium complexes. **G. Elpitiya**, D.M. Jenkins

3:10 INOR **596.** Synthesis of benzoylphosphine via insertion of sodium phosphaethynolate (Na[OCP]) into a zirconium benzyne complex. J. Kieser, R.J. Gilliard, H. Grützmacher, **J.D. Protasiewicz**

3:30 INOR **597.** Hydroboration reactivity of niobium bis(NHC)borate complexes. **J.A. Ziegler**, R.G. Bergman, J. Arnold

3:50 INOR **598.** Planar Ti_2P_2 core assembled by reductive decarbonylation of $^{-}O–C{\equiv}P$. **L. Grant**, B. Pinter, B. Manor, H. Grützmacher, D.J. Mindiola

4:10 INOR **599.** Computational study of extreme π-loading and imido reactivity in CCC-NHC Ta bis(imido) pincer complexes. **C.E. Webster**, G. Liang, T.R. Helgert, J.A. Denny, G.M. Lang, T.K. Hollis

4:30 INOR **600.** Probing Group 4 mixed ligand (Cp, halide, alkoxide) complexes for multiple bonding character and catalytic activity. **N.C. Boyde**, T.P. Hanusa

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Sponsored by PHYS, Cosponsored by INOR

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Mechanistic Studies of Catalysis in Photocatalytic & Photoelectrodes

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

S. A. Koch, *Organizer*

8:00 - 10:00

220-222, 224-226, 229-233, 236, 244, 273, 275-276, 280, 288, 293, 308-309, 319, 323, 328-329, 332-334, 336, 358-359, 362, 365, 379, 382, 384, 388, 390, 394, 396-397, 408-414, 416-418, 422, 424, 429, 440-442, 445, 455, 463, 466, 472, 475, 477, 480, 485-486. See previous listings.

818, 820, 838-843, 846-847, 850-851, 858, 860-864, 880-881, 884, 896, 898, 902-906, 908, 918, 922, 924, 927, 931, 934, 937-938, 941, 947, 949, 952, 954, 961, 967, 968-969, 972, 976, 979-980, 982, 984, 987, 990, 1001-1002, 1004, 1006-1008, 1016-1019, 1021, 1024-1026, 1032, 1034, 1037-1041, 1043-1047, 1051, 1056-1057, 1061-1063, 1066, 1071-1072, 1232. See subsequent listings.

TUESDAY MORNING

Section A

Moscone Center

2009

Gabor A. Somorjai Award for Creative Research in Catalysis: Symposium in honor of John E. Bercaw

N. Hazari, *Organizer*

A. Hazari, *Organizer, Presiding*

8:30 INOR **601.** Thermodynamic efficiency, chemoselectivity and turnover frequency in chemical and electrochemical catalysis: Synergistic principles for catalyst development and optimization. **S.S. Stahl**

8:55 INOR **602.** Recent advances in Ti-catalyzed nitrene transfer reactions. **I. Tonks**, E. Beaumier, H. Chiu, Z.W. Davis-Gilbert, X. See, A.C. Wotal

9:20 INOR **603.** Selective indium and zinc catalysts for controlled polymerization of cyclic esters. **P. Mehrkhodavandi**, T. Ebrahimi, L. Chile, A. Kremer, S. Hatzikiriakos

9:45 INOR **604.** Selective catalytic trimerization of alkenes. **J.A. Labinger**

10:10 Intermission.

10:25 INOR **605.** Cobalt-catalyzed methods for the polyborylation of hydrocarbons. **P.J. Chirik**, N. Palmer, S. Krautwald

10:50 INOR **606.** Group 4 metal complexes for the formation of block copolymers. **P. Diaconescu**

11:15 INOR **607.** Mechanism of formic acid dehydrogenation by a diiridiumtrihydride catalyst. J. Celaje, Z. Lu, E.A. Kedzie, **T.J. Williams**

11:40 INOR **608.** Metal-oxos in chemistry and biology. **H.B. Gray**

12:05 Concluding Remarks.

Section B

Moscone Center
2011

Celebrating 60 Years of the Division of Inorganic Chemistry

Award Winners

M. J. Clarke, *Organizer*

D. C. Crans, *Organizer, Presiding*

K. Bowman-James, K. N. Raymond, *Presiding*

8:00 Introductory Remarks.

8:05 INOR **609.** Synthesis of multinary transition metal chalcogenide nanoparticles for applications in photovoltaics. M. Braun, L. Korala, **A.L. Prieto**

8:35 INOR **610.** Probing anisotropy in molecular magentism. **K.R. Dunbar**

9:05 INOR **611.** Learning from computational studies of NMR chemical shifts: The case of a main group atom in transition metal complex. C. Raynaud, S. Halbert, C. Coperet, **O.G. Eisenstein**

9:35 INOR **612.** Chemical surprises at the frontier of the periodic table. **J.L. Kiplinger**

10:05 Intermission.

10:20 INOR **613.** X-ray spectroscopic studies of biological dinitrogen reduction in molybdenum and vanadium nitrogenases. **S. DeBeer**

10:50 INOR **614.** Pyridinol based ligands for transition metal catalyzed reduction of CO_2 and related substrates: Elucidating the role of Lewis Acids. **E.T. Papish**, S. Siek, D.B. Burks, C. Boudreaux, D.L. Gerlach, G. Liang, D.B. Grotjahn, C.E. Webster

11:20 INOR **615.** Technetium, the first radioelement in the periodic table. **A.P. Sattelberger**, E. Johnstone, M.A. Yates, F. Poineau, K. Czerwinski

11:50 INOR **616.** Design of azurin that spans the entire 2V range of physiological redox potentials and its application in engineering a copper protein that performs fast and reversible S-nitrosylation. **Y. Lu**, P. Hosseinzadeh, S. Tian, J. Liu

Section C

Moscone Center
2016

Undergraduate Research at the Frontiers of Inorganic Chemistry

Bioinorganic Chemistry

A. K. Bentley, C. Nataro, S. R. Smith, *Organizers*

S. A. Toledo, *Presiding*

9:00 INOR **617.** Structural, spectroscopic and reactivity studies of the first structural model of the resting state of Nickel Acireductone Dioxygenase (Ni-ARD). **D. Ivan**, S.A. Toledo, V. Lynch

9:20 INOR **618.** Protein charge effects on Rieske protein reduction potentials. **K.R. Hoke**, A.L. Watkins, R.J. Quarles

9:40 INOR **619.** Modelling the O-O bond formation step in the oxygen-evolving complex. **E. Hanada**, J. Kovacs

10:00 INOR **620.** Trinuclear ruthenium complexes with diimine ligands: Experimental and computational investigations of biological activity. **F.A. Beckford**

10:20 Intermission.

10:35 INOR **621.** Improved photocatalytic activity of hybrid P450 biocatalysts by tuning the Ru(II)-polypyridyl photochemical properties. **H. Shalan**, A. Colbert, T. Nguyen, M. Kato, L.E. Cheruzel

10:55 INOR **622.** Copper transport into the avian oocyte: A second cargo for the vitamin transporter riboflavin binding protein. **S.R. Smith**, M. Benore

11:15 INOR **623.** Photosensitizer-Embedded polyacrylonitrile nanofibers as an antimicrobial non-woven textile. **S. Stanley**, R. Ghiladi

11:35 INOR **624.** Synthesis and conformational analysis of peptides appended to a novel, rigid, cyclic, bimetallic ring system. **T.P. Curran**, A.P. Lawrence, T.S. Murtaugh, W. Ji, N. Pokharel, L.M. Davidson, J.P. Sanderson-Brown, P.R. Handali, V. Nguyen, C. Gober, J. Suitor

11:55 INOR **625.** Rare and unusual square planar copper (I) complexes. **P.A. Cheung**, R. Berger, J.D. Gilbertson

12:15 Concluding Remarks.

Section D

Moscone Center
2018

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of William B. Tolman

L. M. Berreau, *Organizer*

P. L. Holland, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR **626.** Mechanistic studies of Cu(II)/O_2-promoted oxidative aliphatic carbon-carbon bond cleavage reactions. **L.M. Berreau**

9:00 INOR **627.** Reactivity of mononuclear nonheme cobalt(III)-superoxo complexes. **W. Lee**, C. Wang, K. Yeh

9:25 INOR **628.** Bio-inspired heterodinuclear NiFe catalysts for H2 production. D. Brazzolotto, L. Wang, M. Gennari, F. Meyer, M. Orio, V. Artero, **C. Duboc**

9:50 INOR **629.** Why are O_2 and N_2 so different? **K.H. Theopold**, F. Dai, E.S. Akturk, Y. Hung, D.C. Cummins, G.P. Yap

10:15 Intermission.

10:30 INOR **630.** Cu(III) as a biological oxidant? L. Chiang, W. Keown, C. Citek, J.B. Gary, E.C. Wasinger, **T.P. Stack**

10:55 INOR **631.** Modeling nitric oxide signaling chemistry at copper and zinc sites. **T.H. Warren**

11:20 INOR **632.** Studies on the mechanism of Ti-catalyzed nitrene transfer reactions. **I. Tonks**, E. Beaumier, Z.W. Davis-Gilbert, A. Koley, A.J. Pearce, T.A. Wheeler, A.C. Wotal

11:45 INOR **633.** Bioinspired small molecule activation for energy-related catalysis. **F. Meyer**

Section E

Moscone Center
2020

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

Financially supported by Chemistry of Materials

K. R. Kittilstved, E. J. McLaurin, *Organizers*

B. Guiton, K. J. Koski, *Presiding*

8:30 INOR **634.** Chemistry of nanoconfined water molecules in 1-D metal organic nanotubes. **T. Forbes**

9:00 INOR **635.** Fabrication, characterization and application of carbon nanoparticles for the detection of heavy metal ions in aqueous media. **A. Wanekaya**, A.M. Simpson, K. Ghosh

9:30 INOR **636.** Micelle encapsulation: A versatile platform for generating multifunctional nanoparticles. **J.O. Winter**

10:00 Intermission.

10:15 INOR **637.** Novel properties and applications of plasmonic metal nanostructures: A case study and recent progress on Hollow Gold Nanospheres (HGNs). **J.Z. Zhang**

10:45 INOR **638.** Synthesis of Core@Shell nanocatalysts with intermetallic interiors. **S.E. Skrabalak**

11:15 INOR **639.** Controlling nanoscopic and atomic segregation of Pt within Pt-Ni rhombic dodecahedra and nanoframes for fuel cell catalysis. **P. Yang**, N. Becknell, Z. Niu

11:45 INOR **640.** Using nanowire arrays as a sensitive tool for understanding copper-antimony anode materials. E.D. Jackson, **A.L. Prieto**

12:15 Concluding Remarks.

Section F

Moscone Center
2022

Emergent Phenomena in the Solid State

B. C. Melot, *Organizer*

E. E. Rodriguez, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR **641.** Understanding the impact of crystal chemistry on the physical properties of garnets. **B.C. Melot**

9:10 INOR **642.** Mixed-Valence and chemical-pressure effects on magnetic properties of $ThCr_2Si_2$-type pnictides. X. Tan, A. Yaroslavtsev, K. Kovnir, **M. Shatruk**

9:50 INOR **643.** Density functional investigation on the magnetic anisotropy in rare-earth-free metal borides with the $Ti_3Co_3B_2$-type structure. **Y. Zhang**, B. Fokwa

10:10 INOR **644.** Ground state magnetism in S = 1/2 $Li_4MgReO6$ system with orthorhombic crystal structure. J. Milam-Guerrero, C.J. Bloed, P. Nguyen, J.P. Carlo, G. Luke, B.C. Melot, **S. Derakhshan**

10:30 Intermission.

10:50 INOR **645.** Structural and electronic instabilities in electron-doped $Sr_3Ir_2O_7$: Emergent phenomena at the edge of the spin-orbit Mott state. **S. Wilson**

11:30 INOR **646.** Electron doping a kagome spin liquid. **Z. Kelly**, M.J. Gallagher, T. McQueen

11:50 INOR **647.** Magnetic properties of osmium mixed-metal double perovskites. **C. Thompson**, X. Fu

Section G

Moscone Center
2024

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Materials Chemistry of Solutions & Solids for a Sustainable Future

Cosponsored by BMGT‡, MPPG, PRES and PROF‡

J. L. Bryant, J. C. Giordan, *Organizers*

S. E. Hayes, B. L. Maddux, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:40 INOR **648.** Nonlinear optical borates based oxides for solid state laser frequency conversion in the UV range. **G. Aka**, J. Ren, P. Loiseau

9:00 INOR **649.** Atomic solid state energy scale. **J.F. Wager**, D.A. Keszler

9:20 INOR **650.** Chalcogenide semiconductors as p-type transparent conductors, absorbers and alloys. **J. Tate**

9:40 INOR **651.** Characterization of CSMC resists and other nano-material structures: Results and methods. **E.L. Garfunkel**

10:00 Intermission.

10:30 INOR **652.** Solution-Deposition of disordered RuO_2 nanoskins: An example from the fourth quadrant of electronic materials. **D.R. Rolison**

10:50 INOR **653.** New functional materials as a design problem. **A. Zunger**

11:10 INOR **654.** Creating a one-stop platform for computed XAS and NMR materials data and comparison algorithms on the Materials Project. **K. Persson**

11:30 INOR **655.** Solid-state NMR of thin metal oxide films from prompt inorganic condensation. B.A. Hammann, Y. Afriyie, M. Kast, C.K. Perkins, P. Plassmeyer, D.W. Johnson, D.A. Keszler, C. Page, S.W. Boettcher, **S.E. Hayes**

11:50 INOR **656.** Metal-oxo clusters from across the periodic table. **M.D. Nyman**

12:10 INOR **657.** Aqueous inorganic coordination clusters: Synthesis, solution speciation, structure, and their use as inks for materials. **D.W. Johnson**

Section H

Moscone Center
3000

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Cosponsored by BIOL

Financially supported by Northwestern U, U of California-Davis

J. A. Telser, *Organizer*

V. DeRose, *Organizer, Presiding*

8:30 INOR **658.** Cytochrome P450 oxidations: A controlled burn of inert organic compounds. **M. Green**

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

9:00 INOR **659.** Bifunctional peroxidases (KatGs): A challenging family of enzymes for understanding putative evolutionary strategies in fine-tuning the oxidation reactions catalyzed by heme-Trp• intermediates and related e⁻ transfer mediated by Trp•/Tyr•. P.C. Loewen, **A. Ivancich**

9:30 INOR **660.** Mechanistic studies on the radical SAM enzyme CDG synthase. **V. Bandarian**

10:00 INOR **661.** Decoding a secret handshake: Tracking protein-to-protein Cu(I) transfer by rapid x-ray absorption and intrinsic fluorescence techniques. **K.N. Chacon**

10:20 Intermission.

10:30 INOR **662.** How metal ions in the brain tip the toxic balance of the killer prion protein. **G.L. Millhauser**

10:50 INOR **663.** On the use of Co(II) to elucidate Zn(II) enzyme mechanism. **D.L. Tierney**

11:10 INOR **664.** Aromatic amino acid hydroxylases: Exploring the details of a catalytic cycle with EPR spectroscopy. **J.L. McCracken**

11:30 INOR **665.** Taking snapshots of the water oxidation reaction in photosystem II with X-ray crystallography and X-ray spectroscopy. J. Yano, **V.K. Yachandra**

12:00 INOR **666.** Ammonia binding to the OEC of Photosystem II, what does this tell us about water binding and O-O bond formation? **R. Britt**

Section I

Moscone Center

3010

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Conjugated Polymeric Materials

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREM, Argonne National Lab, Northwestern University

A. Facchetti, T. Lohr, *Organizers*

B. M. Savoie, *Presiding*

9:00 Introductory Remarks.

9:05 INOR **667.** Designing responsive piezo-materials from the bottom up: Learning from nonlinear optical materials. **G. Hutchison**, W.S. Horne, C.W. Marvin, H.M. Grimm

9:35 INOR **668.** Polymers and polymer composites for flexible opto-electronic devices. **A. Facchetti**

10:05 INOR **669.** Conjugated polymers and doping strategies for conductive layers and thermoelectric compositions. **H.E. Katz**

10:35 Intermission.

10:45 INOR **670.** Interfacial engineering of two-dimensional nanoelectronic heterostructures. **M. Hersam**

11:15 INOR **671.** Electronic processes, morphologies and structural-functional correlations in low bandgap oligomers and polymers for OPV. **L.X. Chen**

11:45 INOR **672.** Organic polymers for photovoltaics: Small structural differences yield large performance changes. **J.R. Reynolds**

Section J

Moscone Center

3012

Chemistry is Central to Applied Materials

Cosponsored by MPPG‡

C. J. Chang, *Organizer*

C. R. Bertozzi, M. A. Paley, *Organizers*, *Presiding*

8:30 INOR **673.** Dynamic MOF SBUs as active sites for small molecule reactivity and catalysis. **M. Dinca**, E. Metzger, R. Comito, C. Brozek, H. Park, C. Hendon

9:05 INOR **674.** Physical chemistry of nanocrystals with the graphene liquid cell. **P. Alivisatos**

9:40 INOR **675.** Mucin-inspired thermoresponsive synthetic hydrogels induce stasis in human pluripotent stem cell colonies. **S.P. Armes**

10:15 Intermission.

10:30 INOR **676.** Interactions at the nano-bio interface. **C.J. Murphy**

11:05 INOR **677.** Computationally guided discovery of metal-decorated metal–organic frameworks active for catalysis. **L. Gagliardi**, V. Bernales, M.A. Ortuno, A. Mavrandonakis, Z. Li, D. Yang, O.K. Farha, C.J. Cramer, B.C. Gates, J.T. Hupp

11:40 INOR **678.** Grain boundary effects in electroreduction catalysis. **M. Kanan**

Section K

Moscone Center

3001

Switchable Catalysts

J. A. Byers, P. Diaconescu, *Organizers*

A. J. Boydston, A. M. Spokoyny, *Presiding*

8:30 INOR **679.** Switchable catalysis in precision polymerizations in aqueous and organic media. **M. Sawamoto**

9:00 INOR **680.** Organomimetic boron cluster photosensitizers. **A.M. Spokoyny**

9:30 INOR **681.** Stereocontrol in photochemical reactions. **T.P. Yoon**

10:00 INOR **682.** Switchable catalysis in ATRP. **K. Matyjaszewski**

10:30 INOR **683.** Redox-Switchable iron-based polymerization catalysts. **J.A. Byers**, A.B. Biernesser, K.R. Delle Chiaie, J.A. Kehl, M. Qi, A.W. Sudyn

11:00 INOR **684.** Factors controlling the activity of Fe-based catalysts for the polymerization of lactide and epoxides. **C.J. Cramer**, B. Dereli, M. Ortuño

11:30 INOR **685.** Redox-mediated metal-free ring-opening metathesis polymerization. **A.J. Boydston**, L. Pascual, T. Kensy, D. Lee, J. Vandenbrande, N. Alrashdi

12:00 INOR **686.** New avenues in synthesis via organic photoredox catalysis. **D.A. Nicewicz**

Section L

Moscone Center

3003

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

R. Beaulac, W. Feng, *Presiding*

8:00 INOR **687.** Quantifying cation exchange of Cd^{2+} in ZnTe: A challenge for accessing type II heterostructures. **M. Enright**, H. Sarsito, B. Cossairt

8:20 INOR **688.** Room-temperature synthesis of metal chalcogenide nanocrystals from *N*-heterocyclic carbene synthons. **H. Lu**, R.L. Brutchey

8:40 INOR **689.** Design of colloidal semicondutor nanocrystals for enhanced absorption and band edge tuning exceeding 2.0 eV. **D. Kroupa**, M.V. Vörös, N.P. Brawand, B. McNichols, E. Miller, J. Gu, A.J. Nozik, A. Sellinger, G.A. Galli, M.C. Beard

9:00 INOR **690.** Colloidal synthesis of transition metal dichalcogenide nanostructures. **Y. Sun**, Y. Wang, D. Sun, B.R. Carvalho, C. Read, C. Lee, Z. Lin, K. Fujisawa, J.A. Robinson, V.H. Crespi, M. Terrones, R.E. Schaak

9:20 INOR **691.** Design, fabrication and modification of advanced fluorescent polymer based on ordered quantum-dots from nanoscale to large production. **S. Chen**

9:40 INOR **692.** Native phosphine surface ligand exchange on plasma-synthesized indium phosphide nanocrystals. **N.R. Neale**, N.D. Bronstein, L. Wheeler, N.C. Anderson

10:00 INOR **693.** Single-enzyme direct biomineralization of metal chalcogenides nanocrystals with tunable optical properties. **L. Spangler**, Z. Yang, R. Dunleavy, A. Sadeghnejad, R. Chu, L. Lu, C.J. Kiely, B. Berger, S. McIntosh

10:20 Intermission.

10:35 INOR **694.** Synthesis and characterization of colloidal $CsPbX_3$ nanowires. **D. Zhang**, Y. Yang, Y. Bekenstein, Y. Yu, N. Gibson, A.B. Wong, S.W. Eaton, L. Dou, S.R. Leone, P. Alivisatos, P. Yang

10:55 INOR **695.** 2D redox-active superatom frameworks. **A. Champsaur**, C.P. Nuckolls

11:15 INOR **696.** Modulation of electrical and optical properties of tungsten disulfide. **S. Chee**, M. Son, G. Son, H. Jang, M. Ham

11:35 INOR **697.** Chiral semiconductor helices at the mesoscale. **W. Feng**, J. Kim, X. Wang, H.A. Calcaterra, Z. Qu, L. Meshi, N. Kotov

11:55 INOR **698.** Photoredox processes involving colloidal quantum dots: Surface states, structural inhomogeneities, and ultrafast hole extraction. C. Mi, M. Saniepay, P. Dutta, Y. Tang, J.A. McGuire, **R. Beaulac**

12:15 INOR **699.** Synthesis of heterostructured nanocrystals with pre-programmable compositions and spatial arrangements. **X. Li**, R.E. Schaak

Metalloprotein-Initiated Signaling Transduction Response to Redox Stress

Sponsored by BIOL, Cosponsored by INOR

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Applications & Devices

Sponsored by PHYS, Cosponsored by INOR

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Sponsored by NUCL, Cosponsored by INOR and PRES

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Molecular & Bio-Inspired Photocatalysts

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

TUESDAY AFTERNOON

Section A

Moscone Center

2009

Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*

B. Boardman, J. M. Szarko, *Presiding*

1:30 INOR **700.** Highly efficient emitters for Organic Light Emitting Diodes (OLEDs) based on intramolecular rotation and spin-state inversion. **M. Bochmann**, A.S. Romanov, D. Di, L. Yang, D. Credgington, M. Linnolahti

1:50 INOR **701.** Boron containing perovskite single crystal for thermal neutron detection. **M.L. Higgins**, F. Ely, M. Quevedo-Lopez

2:10 INOR **702.** Molecular doping approach for metal oxide photosensitization. **D. Jung**, L.M. Saleh, Z. Berkson, J. Hwang, M.F. El-Kady, E. Titarenko, Y. Shao, K. McCarthy, A.I. Wixtrom, J. Guo, I.B. Martini, S. Kraemer, E.C. Wegener, J. Ciston, J.L. Brosmer, J.I. Zink, J.T. Miller, X. Duan, R.B. Kaner, B.F. Chmelka, A.M. Spokoyny

2:30 INOR **703.** Sensitized Eu^{III} and Tb^{III} emission by functionalized polycarbonate-based materials. **R.A. Tigaa**, X. Aerken, A. Fuchs, A. De Bettencourt Dias

2:50 INOR **704.** Crystal structure effects on the Davydov splitting of electronically active conjugated systems. **J.M. Szarko**, A. Austin, X. Zhu, F.C. Spano, N. Hestand, M. Zdilla

3:10 INOR **705.** Broadband white-light emission in two-dimensional layered lead-bromide perovskites. T. Hu, **M.D. Smith**, E. Dohner, M. Sher, X. Wu, M. Trinh, A. Fisher, J. Corbett, X. Zhu, H. Karunadasa, A. Lindenberg

3:30 Intermission.

3:45 INOR **706.** Micorplasma-assisted synthesis of GQD-AgNP nanohybrids with enhancing light-matter coupling for SERS-based detection. W. Chiang, **K. Lin**

4:05 INOR **707.** Direct polymerization of cobalt chalcogenide clusters for hybrid photovoltaic materials. **B. Boardman**, D.A. Corbin

4:25 INOR **708.** Aiming for the heteroatom control in the synthesis of polyoxometalates. **L. Vilà Nadal**, **J. Mathieson**, **L. Cronin**

4:45 INOR **709.** Luminescent gold(I)-thiophenolate coordination polymers as phase change materials and precursors for the formation of multifunctional nanocomposites. **A. Demessence**, O. Veselska, N. Guillou, M. Monge, G. Ledoux, A. Fateeva, P. Bordet

5:05 INOR **710.** Insulator-to-semiconductor transition in a porous vanadyl Prussian Blue analog upon air exposure. **M. Manumpil**, C. Leal Cervantes, M.R. Hudson, C.M. Brown, H.I. Karunadasa

5:25 INOR **711.** Preparation and properties of tetrathiafulvalene radical cation heavy metal (Pb, Bi) iodide hybrid materials. **H. Evans**, J. Labram, A. Lehner, S. Smock, M.L. Chabinyc, R. Seshadri, F. Wudl

Section B

Moscone Center

2011

Celebrating 60 Years of the Division of Inorganic Chemistry

Recent Officers

M. J. Clarke, D. C. Crans, *Organizers*

B. T. Donovan-Merkert, S. Koch, D. J. Mindiola, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **712.** Bioinorganic systems for artificial photosynthesis. **K. Bren**, S. Chakraborty, P. Lamberg, B. Kandemir, T. Krauss

2:05 INOR **713.** Generation and characterization of primary copper(I)-dioxygen adducts. **K.D. Karlin**

2:35 INOR **714.** Spectroscopic studies of molecular magnetism. **Z. Xue**, S.E. Stavretis, D.H. Moseley, A.A. Podlesnyak, C.M. Brown, L.L. Daemen, Y. Cheng, A.J. Ramirez-Cuesta, X. Wang, C.M. Hoffmann, S.O. Diallo, K. Thirunavukkuarasu, Q. Chen, H. Zhou, J. Ludwig, D. Smirnov, Z. Zhu, M. Guo, J. Tang, H. Cui, F. Fei, X. Chen

3:05 INOR **715.** Coordination chemistry of Fe(II) and Fe(III) MRI contrast agents. **J.R. Morrow**, P.B. Tsitovich, E. Snyder

3:35 Intermission.

3:50 INOR **716.** Synergism of two alkali metals in self-assembly of novel supersized heterobimetallic sandwich compounds. **M.A. Petrukhina**

4:20 INOR **717.** Photomechanical Effects from Ruthenium Sulfoxide Polymers. M. Livshits, J. Shin, **J. Rack**

4:50 INOR **718.** Visible light-induced solid-state CO-releasing compounds. **L.M. Berreau**, S. Anderson, M. Larson

5:20 INOR **719.** Excited state reactivity of transition metal complexes. **C. Turro**

Section C

Moscone Center

2016

Organometallic Chemistry: New Ligand Platforms

Pincer Ligands

N. S. Radu, *Organizer*

O. Ozerov, A. Rahman, *Presiding*

1:30 INOR **720.** Pyrazine-based gold(III) pincer complexes: Synthesis and Luminescence. **J. Fernandez-Cestau**, L. Currie, L. Rocchigiani, B. Bertrand, M. Bochmann, T. Penfold

1:50 INOR **721.** Pincer multifunctionality, together with reduced Fe, cleaves N_2. B.j. Cook, C. Chen, A. Hickey, **K.G. Caulton**

2:10 INOR **722.** New chemistry of pincer-supported rhenium. **A.J. Kosanovich**, W. Shih, O. Ozerov

2:30 INOR **723.** C-H activation and functionalization with PNP rhodium pincers: Stoichiometric reactivity and catalysis. **J. Gair**

2:50 INOR **724.** New insight into C-H borylation with iridium pincer complexes. **O. Ozerov**, L.P. Press, A.J. Kosanovich, C. Lee

3:10 INOR **725.** Bis-N-heterocyclic carbene pincers as versatile ligand platform for uniquely active ester hydrogenation homogeneous catalysts. R. van Putten, G. Filonenko, L. Lefort, E. Hensen, **E. Pidko**

3:30 INOR **726.** Development of new cobalt pincer complexes for catalytic applications. **Y. Li**, **J.A. Krause**, **H. Guan**

3:50 INOR **727.** Iron pincer complexes with isonitrile ancillary ligands for formic acid and methanol dehydrogenation. **N. Smith**, N. Hazari

4:10 INOR **728.** Computational investigation of ester and amide hydrogenation by aliphatic Fe and Ru PNP complexes. **Z. Culakova**, E. Clot, K.I. Goldberg, O.G. Eisenstein

4:30 INOR **729.** Hydrogenation of carboxylic carbonyl derivatives (C=O, C≡N) catalyzed by iron and cobalt pincer complexes or particles. **H. Dai**, J.A. Krause, H. Guan

4:50 INOR **730.** Synthesis and studies of napthaquinone and anthraquinone derived iridium Pincer catalysts for the conversion of ethanol to butanol. **A. Rahman**, W.D. Jones, M. Wiklow-Marnell

5:10 INOR **731.** Synthesis and characterization of new C. C. N Pincer-type palladium complexes containing N-heterocyclic carbene ligands. **J. Yan**, Z. Zhu, Y. Wang, J. Niu, X. Zhu, X. Hao, M. Song

Section D

Moscone Center

2018

ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry: Symposium in honor of William B. Tolman

P. L. Holland, *Organizer*

L. M. Berreau, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 INOR **732.** Nacnac doesn't fall far from the tree: Activation of N_2 with diketiminate complexes. **P.L. Holland**

2:00 INOR **733.** Inorganic chemistry: A salute and a challenge. **R. Eisenberg**

2:25 INOR **734.** Nickel-sulfido and nickel-selenido complexes: Preparation, spectroscopy and C–H activation. **C.G. Riordan**

2:50 INOR **735.** Greater than the sum of their parts: Heterodinuclear polymerization catalysts. **C.K. Williams**

3:15 Intermission.

3:30 INOR **736.** Innovation and potential career paths in industry. **N. Aboelella**

3:55 INOR **737.** Copper transport in methanotrophic bacteria. G.E. Kenney, L.M. Dassama, S.Y. Ro, **A.C. Rosenzweig**

4:20 INOR **738.** Factors controlling the activity of Al-based catalysts for the ring-opening transesterification polymerization of caprolactone. **C.J. Cramer**, B. Dereli, C. Dunbar, J. Freeze, M. Johnson, M. Mandal, D. Marell, H. Vazquez Lima

4:45 INOR **739.** How is metal covalency reflected in ligand field parameters? **F. Neese**, E. Suturina, M. Atanasov

Section E

Moscone Center

2020

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

J. P. Selegue, A. D. Tinoco, *Presiding*

1:30 INOR **740.** Synthesis, characterization and DNA interaction studies of potential anticancer titanium complexes with biologically relevant ligands. **M. Mahroof-Tahir**, **L. Sreerama**, **Z.E. Mahmoud**, **A. Al Dawood**, **E.M. Looli**

1:50 INOR **741.** Inter-duplex distance distributions in metal-modified peptide nucleic acids measured by double electron-electron resonance. **A. Sargun**, A. Jarvi, S.K. Saxena, C. Achim

2:10 INOR **742.** Identifying cancer-relevant DNA damage via a charge transfer mechanism involving [4Fe4S] cluster proteins. **E. Tse**, J.K. Barton

2:30 INOR **743.** Divalent copper complexes as Influenza A inhibitors. **J.D. Lynch**, N.A. Gordon, K.L. McGuire, S.K. Wallentine, G.A. Mohl, R.G. Harrison, D.D. Busath

2:50 INOR **744.** N-Heterocyclic carbene gold(I) complexes conjugated to DNA-aptamers for targeted drug delivery. **W. Niu**, X. Chen, W. Tan, A.S. Veige

3:10 INOR **745.** Regulating photochemistry and nucleic acid targeting of Ru(II) complexes. **P.C. Glazer**

3:30 Intermission.

3:40 INOR **746.** Build-In fluorescent M24L8 octahedral metal organic molecular cages for nuclear-penetrating PH-responsive drug delivery. **Y. Fang**

4:00 INOR **747.** Ruthenium complexes as new pH-dependent switchable metallodrugs. **F. Martinez-Peña**, A.M. Pizarro

4:20 INOR **748.** Expanding the therapeutic potential of the iron chelator deferasirox in the development of aqueous stable Ti(IV) anticancer complexes. **A.D. Tinoco**, S. Loza, A.M. Vázquez, S.C. Perez, Y. Delgado, K. Gaur, K.I. Rivero, L.J. Negron, T.B. Parks, C. Munet-Colon

4:40 INOR **749.** Low-symmetry boron subphthalocyanines as fluorescent imaging probes and precursors for designer metallophthalocyanines. L. Sejdarasi, K. McAuliffe, R. Szlag, M.A. Kaster, **E.R. Trivedi**

5:00 INOR **750.** Mixed polypyridyl/N-heterocyclic carbene complexes as potential cytotoxic pro-drugs. **J.P. Selegue**, R.T. Ryan, J. Mahmoud, P.C. Glazer

5:20 INOR **751.** Targeting ErbB tyrosine kinases with platinum-functionalized small molecule inhibitors. **M. Yang**, H. Wu, T.K. West, C.M. Furdui, G.L. Kucera, U. Bierbach

Section F

Moscone Center

2022

Emergent Phenomena in the Solid State

E. E. Rodriguez, *Organizer*

B. C. Melot, *Organizer, Presiding*

1:30 INOR **752.** Structure and magnetic properties of the 3d transition metal formate-chlorides. **K. Kovnir**

1:50 INOR **753.** Site identity and importance in fluorite-related transparent conductors. **K. Rickert**, A. Dolgonos, **K.R. Poeppelmeier**

2:10 INOR **754.** Withdrawn.

2:50 INOR **755.** Soft chemical control of iron-based superconductors and related compounds. **S. Clarke**

3:30 Intermission.

3:50 INOR **756.** Competing orders in the112 Fe based superconducting family under chemial doping and external pressure. **N. Ni**

4:30 INOR **757.** Hydride route for the synthesis of 122 iron arsenide superconductors. **Y. Zaikina**, M. Kwong, B. Baccam, S. Kauzlarich

4:50 INOR **758.** Layered transition metal chalcogenides based on square lattices as functional materials. X. Zhou, B. Wilfong, H.K. Vivanco, **E.E. Rodriguez**

5:25 Concluding Remarks.

Section G

Moscone Center

2024

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Chemists Leading the Charge: Chemists Using Business Acumen & Transformative Research to Address Societal Needs

Cosponsored by BMGT‡, MPPG, PRES and PROF‡

S. E. Hayes, B. L. Maddux, *Organizers*

J. L. Bryant, J. C. Giordan, *Organizers*, *Presiding*

1:30 INOR **759.** Opening overview: Chemists using business acumen and transformative research to address societal needs. **J.C. Giordan**

‡ *Cooperative Cosponsorship*

1:40 INOR **760.** Importance and value of fundamentally inspired use, use-inspired, and market-informed research. **D.A. Keszler**

2:00 INOR **761.** Science behind oxide transistors for displays. **J.F. Wager**

2:10 INOR **762.** Science behind materials for ink jet printing. **J.E. Abbott**

2:20 INOR **763.** Transformative science behind metal-based EUV photoresists. **S.T. Meyers**

2:30 INOR **764.** Science behind tunneling electronics. **B. Cowell**

2:40 INOR **765.** Interactive panel: Chemists using business acumen and transformative research to address societal needs. **J.C. Giordan**, D.A. Keszler, J.F. Wager, J.E. Abbott, S.T. Meyers, B. Cowell, J.L. Bryant

3:10 Intermission.

3:30 INOR **766.** Opening overview for panel 2: Next generation innovators. **J.C. Giordan**

3:40 INOR **767.** Panel 2: Research to innovation CSMC legacy: Training the next generation. **M. Dolgos**, **J.M. Amador**, **J.C. Ramos**, **J.C. Giordan**

4:10 INOR **768.** Office hours with the speakers. **J.C. Giordan**, D.A. Keszler, J.F. Wager, S.T. Meyers, J.E. Abbott, B. Cowell, M. Dolgos, J.M. Amador, J.C. Ramos, J.L. Bryant

Section H

Moscone Center

3000

Spectroscopic Elucidation of Metalloenzyme Mechanism: Current Successes & Future Challenges

Cosponsored by BIOL

Financially supported by Northwestern U, U of California-Davis

V. DeRose, J. A. Telser, *Organizers*

J. Stubbe, *Presiding*

1:30 INOR **769.** Multifrequency pulse EPR studies of the water oxidizing complex in photosynthesis. **W. Lubitz**, N. Cox, D. Pantazis, F. Neese

2:00 INOR **770.** Progress in high-field EPR and ENDOR spectroscopy to study the radical transfer in class I ribonucleotide reductases. **M. Bennati**

2:30 INOR **771.** Nuclear resonance vibrational spectroscopy as a tool for the characterization of low frequency modes in iron proteins. **V. Schünemann**

3:00 INOR **772.** Nuclear magnetic spectroscopic elucidation of MhuD mechanism. **M.D. Liptak**

3:20 Intermission.

3:30 INOR **773.** Spectroscopic approaches to understanding sulfur insertion into aliphatic carbon centers in the biosynthesis of lipoic acid. **S.J. Booker**

4:00 INOR **774.** Novel outcomes and mechanisms emerging from dioxygen activation by non-heme-di-iron enzymes. **J.M. Bollinger**, C. Krebs

4:30 INOR **775.** Unprecedented [FeS] cluster in the core of the hepatitis B infection. **M. Pandelia**, C. Ueda

4:50 INOR **776.** Elucidating the mechanism and magnetic properties of di-iron-oxo proteins via computational quantum chemistry. **J.H. Rodriguez**

5:10 INOR **777.** Nuclear Resonance Vibrational Spectroscopy (NRVS) of FeFe hydrogenase: New evidence of enzyme intermediates. **S.P. Cramer**

Section I

Moscone Center

3010

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Materials for Energy Conversion

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREM, Argonne National Lab, Northwestern University

A. Facchetti, T. Lohr, *Organizers*

J. R. Reynolds, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **778.** Nitrogen fixation at room temperature, pressure in water using light. **M.G. Kanatzidis**

2:05 INOR **779.** Creation of structurally defined two-dimensional assemblies. **V.P. Conticello**

2:35 INOR **780.** Photosensitization of a CO_2 reduction catalyst with red and near-infrared light using rylenediimide radical anions and dianions. N. LaPorte, J. Martinez, C.M. Mauck, B.T. Phelan, R. Young, **M.R. Wasielewski**

3:05 Intermission.

3:15 INOR **781.** New Polymer Chemistries for Solid Battery Electrolytes. **B.M. Savoie**

3:45 INOR **782.** Solution-processed metal oxide materials for large-area flexible electronics and hydrogen energy devices. **M. Yoon**

4:15 INOR **783.** Novel synthetic approaches for efficient semiconducting materials. **A. Dudnik**

Section J

Moscone Center

3012

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

B. Baruah, Y. Zhou, *Presiding*

1:30 INOR **784.** Porous benzoxazoles as oxygenation catalysts: Case of amine self-coupling. S. Subramanian, H.A. Patel, Y. Song, **C.T. Yavuz**

1:50 INOR **785.** High power factor and enhanced thermoelectric performance of SnTe: Synergistic effect of resonance level and valence band convergence. **K. Biswas**

2:10 INOR **786.** Diffusion of cations in 2D/3D perovskite films made by melt infiltration. **E. Keenan**, J. Hu, J. Zhi, D.B. Mitzi, W. You

2:30 INOR **787.** New 2D hybrid perovskite systems for optoelectronic applications. **C. Lermer**, S.T. Birkhold, S.P. Harm, I.L. Moudrakovski, L.M. Schoop, P. Mayer, L. Schmidt-Mende, B.V. Lotsch

2:50 INOR **788.** Stabilization of the metastable perovskite phase of Formamidinium Lead Triiodide ($FAPbI_3$) *via* surface functionalization. **Y. Fu**, J. Zhai, M. Shearer, S. Jin

3:10 INOR **789.** Interfaces and their influence on oxide ion diffusion in ceria. **A.K. Lucid**, G.W. Watson

3:30 Intermission.

3:45 INOR **790.** Engineering carbon sheets supported iron nanoparticles for direct synthesis of light olefins. **Y. Zhou**, C. Wang, S. Natesakhawat, J. Leske, D. Kauffman, C. Matranga

4:05 INOR **791.** Cotton fabric immobilized ZnO@AuNP for heterogeneous catalysis. **B. Baruah**, D. Agyeman, S. Baruah

4:25 INOR **792.** Structural informatics: Its role in understanding metal-organic complexes. **S. Vyas**, A. Sarjeant

4:45 INOR **793.** Charge density mismatch synthesis and application to UZM-35, a material containing both 10MR and 12MR pores. **C.P. Nicholas**

5:05 INOR **794.** Advancing marine hydrokinetic energy technology through materials chemistry. **B.A. Hernandez-Sanchez**, M.R. Hibbs, P.B. Savage

5:25 INOR **795.** Hierarchical structured MnO_2 nanoparticle-embedded SiO_2 nanofibrous membranes with flexibility and enhanced catalytic performance. **D. Lvye**, X. Wang, R. Zhang, B. Ding

Section K

Moscone Center

3001

Switchable Catalysts

J. A. Byers, P. Diaconescu, *Organizers*

C. Chen, B. K. Long, *Presiding*

1:30 INOR **796.** ROP of β-lactones: From syndiotactic homopolymers to blocky and chemically tunable alternating copolymers. C. Jaffredo, R. Ligny, S.M. Guillaume, **J. Carpentier**

2:00 INOR **797.** Cationic indium catalysts for formation and polymerization of functionalized monomers. **P. Mehrkhodavandi**, I. Yu, C. Chang, C. Diaz Lopez

2:30 INOR **798.** Exploring the chemical space of redox-switchable catalysts. **N. Fey**, P. Diaconescu

3:00 INOR **799.** Rare-earth metal-based catalysts for ring-opening polymerization of lactide monomers. **J. Okuda**

3:30 INOR **800.** Lewis acid and redox control in olefin polymerization. **C. Chen**

4:00 INOR **801.** Modulating polyolefin microstructure and composition via redox-active catalysts. W.C. Anderson, J. Kern, S. Roy, **B.K. Long**

4:30 INOR **802.** Design and development of metal-free light controlled polymer systems. **J. Read De Alaniz**

5:00 INOR **803.** Stereo- and temporal switch coordination polymerization of conjugated dienes and styrene. **D. Cui**, B. Liu, C. Yao

Section L

Moscone Center

3003

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

N. J. Deyonker, A. R. O'Connor, *Presiding*

1:30 INOR **804.** Catalytic and mechanistic evaluation of norbornene polymerization initiated by cationic (π-Allyl) group 10 complexes containing dialkylbiaryl phosphine ligands. **A.R. O'Connor**, C. Lee, M. Kunitomo, N.B. Jones, G.L. Heard

1:50 INOR **805.** Palladium-catalyzed hydrophosphorylation of alkynes: Scope, limitation and mechanism. **L. Han**

2:10 INOR **806.** Can alkylation of the N–H functionality within M/NH bifunctional Noyori-type catalysts lead to improved activity? **P.A. Dub**, J.C. Gordon

2:30 INOR **807.** Hydroarylation of olefins with (pyridyl-indole) Pt^{II} complexes. **B.A. Suslick**, A.L. Liberman-Martin, T.D. Tilley

2:50 INOR **808.** Mechanistic elucidation of Pd-catalyzed reactions using high resolution electrospray ionization mass spectrometry. **K.L. Walker**, L.M. Dornan, M.J. Muldoon, R.N. Zare, R.M. Waymouth

3:10 INOR **809.** Polymer-supported palladium (II) carbene complexes: Catalytic activity, recyclability and selectivity in C–H acetoxylation of arenes. **M.H. Majeed**, **P. Shayesteh**, **R.L. Wallenberg**, **A.R. Persson**, **N. Johansson**, **L. Ye**, **J. Schnadt**, **O.F. Wendt**

3:30 INOR **810.** Mechanism of Pd-catalyzed decarbonylation of esters to linear α-olefins. **M.A. Ortuno**, B. Dereli, A. John, H.E. Johnson, M.A. Hillmyer, W.B. Tolman, C.J. Cramer

3:50 INOR **811.** Modeling the selectivity of the Pd-based hydroxycarbonylation of pentenoic acids to adipic acid. B. Pudasaini, **A. Genest**, N. Roesch

4:10 INOR **812.** Is an exhaustive conformational search necessary for proposing catalytic mechanisms? An investigation of intramolecular Heck catalysis in the formation of colletoic acid derivatives. **N.J. Deyonker**, T. Ling, R.N. Waltman, F. Rivas

4:30 INOR **813.** Solvent influence into the C_{sp2}-X (X= Cl o Br) bond activation of x-pyridine species by neophylpalladacycle: An experimental study. **O. Serrano**

4:50 INOR **814.** Mechanistic study of the bis(trineopentylphosphine)palladium catalyzed Buchwald-Hartwig amination reaction. **H. Hu**, K.H. Shaughnessy

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Theory & Modeling

Sponsored by PHYS, Cosponsored by INOR

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Sponsored by NUCL, Cosponsored by INOR

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Sponsored by NUCL, Cosponsored by INOR and PRES

Deposition & Etching of Nanostructures

Sponsored by COLL, Cosponsored by INOR

Support & Activator Effects on Metal Mediated Polymerization

Sponsored by PMSE, Cosponsored by CATL, INOR and MPPG‡

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Novel Photocatalytic & Photoelectrode Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

TUESDAY EVENING

Section A

Moscone Center
Hall D

Inorganic Spectroscopy

V. C. Popescu, *Organizer*

5:30 - 7:30

INOR **815.** Influence of charge transfer in the photoluminescence of lead-free $Ba_{1-x}Ca_xTi_{0.9}Zr_{0.1}O_3$ electro-ceramics. **G. Herrera Pérez**, J.G. Murillo, G. Zaragoza-Galán, G. Tapia-Padilla, A. Reyes-Rojas, L.E. Fuentes-Cobas

INOR **816.** Characterizing the inner filter effect in quantum dot-polymer composites for use as a displacement sensor. **M.A. Koc**, P. Alivisatos

INOR **817.** Single-molecule investigation of initiation dynamics of an organometallic catalyst. **J. Ng**, S. Upadhyay, A. Marquard, K. Lupo, D. Hinton, N. Padilla, D. Bates, R.H. Goldsmith

INOR **818.** Mössbauer spectroscopy: Predictive property models from experimental design and statistical learning. **J. Proppe**, M. Reiher

INOR **819.** Measuring of the energy transfer efficiency between plasmon nanoparticles and quantum dots using Sample-Transmitted Excitation Photoluminescence (STEP). **P. Moroz**, M. Zamkov

INOR **820.** Withdrawn.

INOR **821.** Photophysical effects of varying imine based ligands with cuprous halides to form vividly-colored/brightly-phosphorescent coordination polymers. **L.E. Scoggins**, M. Wilk, Z. Henry, V. Nesterov, M. Omary

INOR **822.** TDDFT studies of earth abundant photocatalysts. **C. Nite**, A.K. Rappe

INOR **823.** Theoretical study of tris(1,3-propanedionato)chromium(III) for insight into Cr(III)-based photocatalysts. **J. Nite**, A.K. Rappe

INOR **824.** Thermal polarized vibrational microspectroscopy of weddellite and whewellite single crystals. **G. Kumi**, N. Aljuhani, A. Obaid

INOR **825.** Mössbauer spectroscopy of iron-selone and and iron-thione complexes capable of preventing oxidative DNA damage. **V.C. Popescu**, M. Cohara, J.L. Brumaghim, B. Stadelman

INOR **826.** Reexamination of the red band of CuO: Analysis of the [16.5] $^2\Sigma^- - X\ ^2\Pi_i$ transition of ^{63}CuO and ^{65}CuO. **J.C. Harms**, E.M. Grames, S. Yun, B. Ahmed, J.J. OBrien, **L.C. O'Brien**

INOR **827.** Analysis of some new electronic transitions observed using intracavity laser spectroscopy (ILS): Possible Identification of HCuN. **J.C. Harms**, E.M. Grames, J.J. OBrien, L.C. O'Brien

INOR **828.** XESCA: X-ray emission spectroscopy for chemical analysis. **S. Lee**

Section B

Moscone Center
Hall D

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

5:30 - 7:30

INOR **829.** Highly selective and sensitive colorimetric chemosensor for detection of Co^{2+} in a near-perfect aqueous solution. **M. Kim**, H. Cho, C. Kim

INOR **830.** Colorimetric chemosensor for the sequential recognition of mercury (II) and iodide in aqueous media. **H. Ahn**, S. Hwang, M. Yang, C. Kim

INOR **831.** Simultaneous bioimaging recognition of cation Al^{3+} and anion F^- by a fluorogenic method. **J. Kang**, H. Jeong, D. Yun, C. Kim

INOR **832.** Highly sensitive benzimidazole-based chemosensor for the colorimetric detection of Fe(II) and Fe(III) and the fluorometric detection of Zn(II) in aqueous media. **H. Jang**, J. Chae, A. Kim, C. Kim

INOR **833.** Highly selective fluorescence sensor for Al^{3+} and CN^- in aqueous solution: Biological applications and DFT calculations. **J. Jung**, J. Yun, P. Kim, C. Kim

INOR **834.** Pillarplexes: A metal-organic class of supramolecular hosts. **P.J. Altmann**, A. Pöthig

INOR **835.** Unprecedented metal-ligand cooperation of a (PPP)Ni scaffold: Formation of P-E bonds (E = N or P). **Y. Kim**, Y. Lee

INOR **836.** Frist-row metal complexes of poly(guanidinyl)aryl ligands. J.E. Allen, L. Wilkinson, W.S. Kassel, **N.A. Piro**

INOR **837.** Solvent free hydrosilylation of tertiary, secondary and primary amides using BIAN [Bis(Arylimino)-Acenaphthene] based Iron complexes. **A. Saini**, M. Findlater

INOR **838.** Synthesis of a novel multitopic nonchelating N-heterocyclic carbene. **D. Tapu**, **A. Carter**, **R. Justice**, **R. Hooper**, O. Kuykendall, M. Baker, G. Bettler, A. Changas, A. Mason

INOR **839.** New annulated N-heterocyclic carbenes and their transition metal complexes. **G. Bettler**, **A. Changas**, O.J. Buckner, C. Boudreaux, B. Norvell, D. Tapu

INOR **840.** Toward the synthesis of a new anionic N-heterocyclic carbene and its corresponding metal complexes. **A. Carter**, **A. Mason**, **D. Tapu**, M. Baker, G. Bettler, A. Changas

INOR **841.** Synthesis and Characterization of Cr(0) terminated π-linkers based on linear oligoazulenic frameworks. **N.R. Erickson**, M.V. Barybin

INOR **842.** Hetrobimetallic complexation of a mercapto and isocyano functionalized linear 6,6'-biazulenic π-linker: Synthesis, redox behavior, and spectroscopic characterization. **J.C. Applegate**, N.R. Erickson, M.V. Barybin

INOR **843.** Novel mesoionic/remote N-heterocyclic carbene ligands and their ruthenium(II) aqua complexes. **T.C. Cao**, D.B. Grotjahn

Section C

Moscone Center
Hall D

Main Group Chemistry

T. W. Hudnall, *Organizer*

5:30 - 7:30

INOR **844.** Aluminium carboxylates as precursors for the synthesis of aluminium-oxo-cages. **T.L. Precht**, A.J. Peel, D. Wright, A. Wheatley

INOR **845.** Reactivity of an acyclic silylsilylene toward ethylene: Migratory insertion into the Si-Si bond. **D. Wendel**, S. Inoue, B. Rieger

INOR **846.** Borylated N-Hetereocyclic Carbenes(NHCs) - Synthesis and migration studies. **W. Liu**, C. Chiu

INOR **847.** Synthesis and characterization of energetic nitroformate salts. **A. Baxter**, I. Martin, K.O. Christe, R.M. Haiges

INOR **848.** Triazenyl radicals stabilized by *N*-heterocyclic carbenes. **J. Back**, E. Lee

INOR **849.** Silylene stabilized boron cations: Synthesis and reactivity studies. **H. Tsai**, C. Chiu

INOR **850.** Acid-catalyzed hydroxylation of iodododecaborate. **Z.S. Lincoln**, J.A. Dopke, R.J. Staples

INOR **851.** Ruthenium-catalyzed substitutions of icosahedral dodecaborates. **D.C. Adams**, J.A. Dopke, R.J. Staples

INOR **852.** Synthesis and characterization of salts derived from 5[chloroalkly]tetrazoles. **Y.O. Ahmed**, C. Gibson, S. Schneider, S. Deplazes

INOR **853.** Synthesis and characterization of new derivatized 1,1dimethylhydrazinium salts. Y.O. Ahmed, **C. Gibson**, S. Schneider, S.F. Deplazes

INOR **854.** Withdrawn.

INOR **855.** Polyphosphazenes as antibacterial films. **P. Nance**, P. Wisian-Neilson

INOR **856.** Stabilization of heavier main group analogues by London dispersion force interactions. **R.E. Tureski**, P.P. Power

Section D

Moscone Center
Hall D

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

5:30 - 7:30

INOR **857.** 1,3,6-Trisubstituted fulvene derived *ansa*-metallocene ligands: A new route for the synthesis of *ansa*-ytterbocenes and –samarocenes. **S.K. Adas**, G.J. Balaich

INOR **858.** Cyclopentadienyl pyridazines and oxazines and their applications in energy and advanced electronics. **N.C. Tice**, E.M. Collins, C.A. Snyder, D.L. Smith

INOR **859.** Influence of the dicopper core on the reactivity of copper(I) hydrides. **A.J. Jordan**, P.K. Thompson, C.M. Wyss, J.P. Sadighi

INOR **860.** Unusual reactivity of PCP-supported rhenium carboxylates. **A.J. Kosanovich**, W. Shih, O. Ozerov

INOR **861.** Activation of small molecules by 2-[(dicyclohexylphosphino)ethyl] trimethyl ammonium chloride iridium complexes. **J. Knapp**, S.H. Schreiner

INOR **862.** Comparative reactivity studies of iridium(I) and rhodium(I) complexes stabilized by chelating diphosphine ligands. **K. Olsen**, S.H. Schreiner

INOR **863.** Synthesis, characterization and reactivity of group ten phosphinoferrocene - carbonyl complexes. **E. Kober**, S.H. Schreiner

INOR **864.** Synthetic and structural comparisons between first row transition metal dithiolato complexes and group 14 metalylenes. **J. Pratt**, P.P. Power

Section E

Moscone Center
Hall D

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

5:30 - 7:30

INOR **865.** Single step access to long-chain α,ω-dicarboxylic acids by catalytic isomerizing hydroxycarbonylation. **V. Goldbach**, L. Falivene, L. Caporaso, L. Cavallo, S. Mecking

INOR **866.** Carbon dioxide hydrosilylation catalyzed by iron. **T. Jurado**, J.J. Garcia

INOR **867.** Robust catalyst for the dehydrogenation of neat formic acid. J. Celaje, Z. Lu, **E. Kedzie**, J. Lo, N. Terrile, T.J. Williams

INOR **868.** Olefin oligomerization catalysis: Ligand design, organometallic chemistry, and catalysis. **T.C. Wambach**, T.D. Tilley

INOR **869.** Ammonia formation from a bulky triphenolate amine transition-metal nitrido complex. **D. Bae**, E. Lee

INOR **870.** 1,5-Regioisomer of the click reaction: Valuable ligand precursors for new Ru-MIC complexes. **L. Suntrup**, S. Hohloch, B. Sarkar

INOR **871.** Computational studies of rhodium-catalyzed hydrogenation and carbon dioxide activation. **M. Trenerry**, M.T. Whited, B.L. Taylor

INOR **872.** Hydrogenation of unsaturated triglycerides via catalytic hydrogen transfer from glycerol. **V. Cherepakhin**, T.J. Williams

INOR **873.** Highly efficient synthesis of *N*-alkylation of aromatic amines with primary alcohols catalyzed by an ionic ruthenium pincer complex. F. Yang, Y. Wang, Y. Ni, X. Cao, S. Lu, **X. Hao**, M. Song

INOR **874.** Synthesis and electrochemistry of ruthenium 2,2'-bipyridine-6,6'-dicarboxylate catalysts using different phosphorus ligands. **S. Yazdani**, J.M. Kamdar, E.R. Paulson, A.L. Rheingold, D.B. Grotjahn

INOR **875.** Kinetic investigation of the dehydrogenative borylation of terminal alkynes. **B.J. Foley**, N. Bhuvanesh, O. Ozerov

INOR **876.** Tunable catalysis with dimetal tetraguanidinate paddlewheel complexes. **M. Humphries**, E. Wusterbarth, B.R. Smith, J.T. Njardarson, D.L. Lichtenberger

INOR **877.** Catalytic aerobic oxidation by self-sensitized tellurium containing chromophores. **L. Lutkus**, T. McCormick

INOR **878.** Reactivity and catalytic studies of transition metal complexes with a triazenide ligand functionalized with pyrazole. **L.J. Medrano-Castillo**, M.Á. Collazo-Flores, D. Chávez, D.B. Grotjahn, A.L. Rheingold, V. Miranda-Soto, M. Parra Hake

INOR **879.** Butterfly [2Fe-2S] cluster-based electrocatalysts with fast rates for hydrogen production. **K.E. Clary**, O. In-noi, J.M. Marx, K.J. Haller, D.H. Evans, R.S. Glass, D.L. Lichtenberger

‡ *Cooperative Cosponsorship*

INOR **880.** Rhodium complexes with N-heterocyclic carbene and triazenide ligands as catalysts for alkyne hydrothiolation. **J.P. Camarena-Díaz**, D.B. Grotjahn, A.L. Rheingold, J. Perez-Torrente, R. Castarlenas, L.A. Oro, V. Passarelli, M. Parra Hake, V. Miranda-Soto

INOR **881.** Oxidation of an iridium hydride pincer complex by O_2: A DFT study. **J. Williams**, A.M. Wright, K.I. Goldberg, T.R. Cundari

INOR **882.** Development of novel Pd and Pt catalysts for efficient conversion of methane to methanol. **J. Chen**, **J. Park**, **M. Klosinski**, R. Giron, Y. Lee, B. Rawal, J. Lee, K.W. Jung

Section F

Moscone Center

Hall D

Inorganic Catalysts

S. A. Koch, *Organizer*

5:30 - 7:30

INOR **883.** Olefins from biodiesel: Decarbonylation using a ruthenium catalyst. **B. Benson**, A. John, W.B. Tolman

INOR **884.** Reduced copper metal-organic frameworks: A heterogeneous catalyst for click chemistry. **K. Xie**, Q. Fu, P. Webley, G.G. Qiao

INOR **885.** Study on synthesis and catalytic cracking performance of Y zeolite with sheet-like morphology. **S. Cui**, G. Wang, B. Liu

INOR **886.** Copper nanocrystals embedded in metal-organic frameworks for highly selective CO_2 hydrogenation to methanol. **B. Rungtaweevoranit**, J. Baek, G.A. Somorjai, O.M. Yaghi

INOR **887.** Mesoporous cobalt oxide with controlled porosity: Efficient catalyst for peroxide free alkene epoxidation under aerobic conditions. **C. Weerakkody**, S.L. Suib

INOR **888.** Copolymerization of cyclohexene oxide and succinic anhydride using Schiff base Zn complex. **A. Virachotikul**, P. Wongmahasirikun, K. Phomphrai

INOR **889.** Synthesis of cyclic poly(ε-caprolactone) using tin(II) complex containing soft sidearm initiator. **T. Ungpittagul**, K. Phomphrai

INOR **890.** Investigation of ring-opening mechanism using x-ray crystallography. **K. Udomsasporn**, K. Phomphrai

INOR **891.** Cobalt, nickel, and iron Schiff Base complexes for hydrogen production in aqueous solution. A. Graves, O. Taghavi, **W.T. Eckenhoff**

INOR **892.** Synthesis of aluminum complexes supported by salicylaldimine ligands for the polymerization of cyclic esters. **P. Pisitsopon**, P. Wongmahasirikun, K. Phomphrai

INOR **893.** Electrocatalytic generation of hydrogen gas by cobalt porphyrin-based Metal-Organic Framwork (MOF) and amorphous polymer. **Y. Wu**

INOR **894.** Studies of a low-valent Molybdenum(VI)-dioxo complex as a deoxydehydration catalyst. **R. Tran**, S.M. Kilyanek

INOR **895.** Novel bi-functional catalyst based on Co_3O_4 core – MnO_2 shell for rechargeable Li–air battery. **Y. Lee**, D. Kim, S. Ha, S. Kim, **Y. Lee**

INOR **896.** Impact of rare-earth dopants on the catalytic activity of CeO2 nanoparticles for both CO oxidation and preferential CO oxidation reactions. **J. Yoo**, K. Kim, J. Han, W. Jung

INOR **897.** Aqueous solution palladium catalyzed Suzuki cross coupling reactions: Reaction optimization of base and the effects of base concentration. **T. Olson**, J.G. Parsons

INOR **898.** Effects of acid strength and position of an intramolecular acidic functional group on the catalytic reduction of CO_2 to CO. **S. Lense**, I.A. Guzei, K. Thao, J. Andersen, M. Schultz

INOR **899.** Inverse Frustrated Lewis Pair (FLP) approach for catalytic metal-free hydrogenation of imines. **S. Mummadi**, D. Kenefake, R. Diaz, C. Krempner

INOR **900.** Role of water in the selective oxidation of benzyl alcohol over gold nanoparticle supported catalysts. **A. Tombo**, M.Y. Santos, B. Chandler, C. Pursell

INOR **901.** Withdrawn.

INOR **902.** Withdrawn.

INOR **903.** Characterizing the kinetic capabilities of supported gold nanoparticle catalysts using benzyl alcohol oxidation. **M.Y. Santos**, B.D. Chandler, C. Pursell, A. Tombo

Section G

Moscone Center

Hall D

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

5:30 - 7:30

INOR **904.** Impedance studies of silyl/carbonate electrolyte blends. **M. Treichel**, **C.A. Ortiz**, L.J. Lyons

INOR **905.** Nitrous oxide removal with titanium oxide. **H. Gokturk**

INOR **906.** Synthesis and characterization of magnetic nanocomposites for energy storage applications. **B. Shen**, S. Sun

INOR **907.** Development of a chemosensor device to aid in combatting the trade of fish caught by cyanide fishing. **C. Flynn**, **C.A. Sweet**, A.R. McCabe, C. Murphy

INOR **908.** Design of biotemplated titanium dioxide nanoparticles for potential application as anodes in dye-sensitized solar cells. **A. Reyes-Oliveras**, G. De Jesus-Morales, V. López-Mejías

INOR **909.** Photophysical studies on homoleptic phenylimidazolinato Ir(III) complexes: Electronic effect of terphenyl groups at the phenylimidazolinato ligand. **S. Kim**, Y. Cho, C. Kim, H. Son, S.O. Kang

INOR **910.** New types of deep blue phosphorescent Ir complexes with sulfonyl group in phenyl unit of phenyl pyridine ligand: Photodynamic studies of sulfonyl group effect and their application to solid-state display. **J. Kim**, Y. Cho, S. Yi, C. Kim, H. Son, S.O. Kang

INOR **911.** Iridium photosensitizers for artificial photosynthesis: Design monomeric and bimetallic Ir-complexes and Ir-dendrimers. **Y. Cho**, C. Kim, H. Son, C. Pac, S.O. Kang

INOR **912.** Widely controllable syngas (H_2 + CO) production by a dye-sensitized TiO_2 hybrid system with Re(I) and Co(III) dual molecular catalysts under visible-light irradiation. **J. Lee**, D. Won, W. Jung, H. Son, C. Pac, S.O. Kang

INOR **913.** Role of porphyrin antenna for photocatalytic CO_2 reduction in a hybrid catalyst system: Protection from photo-bleaching. **D. Won**, J. Lee, H. Son, C. Pac, S.O. Kang

INOR **914.** Photosensitization effects of Ir(III) complexes in selective reduction of CO_2 by Re(I)-complex-anchored TiO_2 hybrid catalyst. H. Cheong, S. Kim, Y. Cho, D. Cho, C. Kim, **H. Son**, C. Pac, S.O. Kang

INOR **915.** Photophysical studies on homoleptic phenylimidazole iridium(III) complexes: Electronic effect of planar bulky phenylimidazole ligand. **M. Son**, S. Kim, Y. Cho, J. Kim, S. Yi, C. Kim, H. Son, S.O. Kang

INOR **916.** Molecular engineering of squaraine dyes for efficient far-red and near-IR sensitization in photocatalytic CO_2 reduction. **M. Cho**, H. Son, C. Pac, S.O. Kang

INOR **917.** Measuring lithium and fluorine diffusion in electrolytes for use in lithium-ion batteries with PFG-STE NMR. **S.A. Beecher**, L.J. Lyons

INOR **918.** Coupling of chromophoric dyes with applied bias or microwave heating to increase DSSC photoconversion efficiency. **C.A. Sweet**, **C. Flynn**, C.J. Timpson, C. Murphy

INOR **919.** Effect of aliphatic ligand length on triplet energy transfer from PbSe nanoparticles to rubrene. **N. Megerdich**, M. Mahboub, M. Tang

INOR **920.** Structure, dynamics, and electrochemistry of psychrophilic cytochromes. **S.J. Barth**, **J. Chou**, **S.K. Lone**, **K.S. Montero**, **G.J. Salerno**, **M.C. Buzzeo**, **J.S. Magyar**

INOR **921.** Bioinispired preparation of melanin-like nanoparticles used for highly nitrogen-doped porous carbon spheres: Enhanced CO_2 capacities and efficient oxygen reduction catalyst. H. Kim, M. Kim, M. Kang, Y. Sung, **W. Yoo**

Section H

Moscone Center

Hall D

Electrochemistry

B. L. Lucht, *Organizer*

5:30 - 7:30

INOR **922.** Vanadium oxide and vanadium oxynitride composite as electrode materials for lithium ion batteries. **W. Huang**, S. Yen, C. Lee, H. Chiu

INOR **923.** Synthesis, characterization and electrocatalytic performance of binary transition metal borides. **H. Park**, B. Fokwa

INOR **924.** Exploring electrocatalytic N_2 activation under mild synthetic conditions. **A. Nielander**, J. McEnaney, T.F. Jaramillo

INOR **925.** Rutile TiO_2 Nanorod arrays grown on graphite foil as binder-free flexible electrode for sodium-ion batteries. **Y. Ching Tai**, M. Yang, H. Chiu, C. Lee

INOR **926.** Molecular rectification: Chemical synthesis and characterization of donor-sigma-acceptor molecules. G. Ren, E.J. Parish, **H. Honda**, H. Shyu, T. Wei

INOR **927.** Characterization of a dicopper dihydroxide water oxidation electrocatalyst. **S.J. Koepke**, P.E. VanNatta, A. Shrestha, M.T. Kieber-Emmons

INOR **928.** Electrochemical characterization of selenocystine reactivity at modified gold surfaces. **K. Frommer**, **K. Lynch**, **E. Wiita**, **M.C. Buzzeo**

INOR **929.** Withdrawn.

Section I

Moscone Center

Hall D

Bioinorganic Chemistry: DNA, RNA & Inorganic Drugs

S. A. Koch, *Organizer*

5:30 - 7:30

INOR **930.** Elucidation of the cell death pathways induced by aqueous-stable titanium(IV) compounds as potential anticancer agents. **Y. Delgado**, A.D. Tinoco

INOR **931.** Glycoconjugates of organometallic ruthenium-arene complexes. **L. Miller**, **L. Kennington**, L. Wisniewski, M. Burnatowska-Hledin, A.L. Eckermann

INOR **932.** Synthesis, characterization, and in-vitro antitumor activity of copper(II) complexes possessing alky-substituted polypyridyl ligands. **J.F. Eichler**, N. Angel, M. Baird, R.M. Khatib

INOR **933.** Functionalised peptidomimetic metallohelices. **H. Song**, S. Allison, S. Shepherd, R. Phillips, P. Scott

INOR **934.** Photodynamic therapy of cancer using sterically strained ruthenium complexes. R.S. Khnayzer, N. Mansour, S. Mehanna, R.I. Taleb, M. Mroueh, M. ElSibai, **C.F. Daher**

INOR **935.** Design, synthesis and characterization of multifunctional platinum-[benz] acridine agents. **X. Yao**, M.W. Wright, M. Yang, J. Lee, C.M. Furdui, U. Bierbach

INOR **936.** Synthesis, characterization, and binding properties of metal-based G4 intercalators containing a phosphonium tether. **G.M. Marqus**, M. Dixon, M. Powers, C.H. Leung

INOR **937.** Fluorinated pyrrolic macrocycles for biological imaging: Optical properties and aggregation in solution. **M.A. Kaster**, R. Szlag, K. McAuliffe, E.R. Trivedi

INOR **938.** Rhenium-oxo and gold corroles: Synthesis, spectroscopy, and application to photodynamic therapy. **R.F. Einrem**, A. Alemayehu, O.A. Gederaas, **A. Ghosh**

INOR **939.** Synthesis and application of silver nanoclusters from DNA templates containing Ag(I)-mediated base pairs. **J. Léon**, D. Gonzalez-Abradelo, G. Wilde, M. Peterlechner, C. Strassert, J. Müller

INOR **940.** From cations to clusters: Ag^+-mediated DNA base pairings and fluorescent silver clusters. **S. Swasey**, X. Chen, A. Karpenko, S.M. Copp, O. Lopez-Acevedo, E. Gwinn

INOR **941.** Acid-labile linker design for targeted delivery and release of platinum-acridine anticancer agents. **H. Wang**, M. Yang, U. Bierbach

INOR **942.** Anticancer properties of organorhenium picolinato, nicotinato and tryptophanato complexes. **M. Stevenson**, S. Pramanik, S.K. Mandal

INOR **943.** Cytotoxic properties of organorhenium flufenamato and ibuprofenato complexes on breast cancer cells. **S. Parnell**, S. Pramanik, S.K. Mandal

INOR **944.** Anticancer properties of organorhenium mefenamato and tolfenamato complexes. **T. Hinton**, S. Pramanik, S.K. Mandal

INOR **945.** Chemical biology of Cu(II) complexes with imidazole or thiazole containing ligands: Synthesis, crystal structures and comparative biological activity. **L.A. Tyler**, A. Lewis, M. McDonald, S. Scharbach, S. Hamaway, K.M. Fox, J. Tanski, L. Cassimeris

Section J

Moscone Center
Hall D

Bioinorganic Chemistry: Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

5:30 - 7:30

INOR **946.** Square planar copper (I) complexes with geometric constraints pertinent to copper proteins. **P. Cheung**, R. Berger, J.D. Gilbertson

INOR **947.** Synthetic models of Ni-thiolate coordination units in biology. **R.A. Steiner**, T.C. Harrop

INOR **948.** Electronic ground state determination of a novel paramagnetic iron(III)-superoxo complex by Mössbauer spectroscopy, EPR, and DFT. **H. Stout**, S.T. Kleespies, C. Chiang, W. Lee, L. Que, E. Munck, E.L. Bominaar

INOR **949.** Electronically versatile benzenedithiolates on electronic and coordination structures of metal complexes: Mimicking the electronic interplay in [FeFe]hydrogenase active site. **Y. Liu**, K. Chu, M.H. Chiang

INOR **950.** Withdrawn.

INOR **951.** Nitrite reduction by a PDI complex with a proton-responsive secondary coordination sphere. **M. Delgado**, Y.M. Kwon, J.D. Gilbertson

INOR **952.** Probing Pterin reduction dynamics in synthetic molybdenum cofactor models. **A.L. Nagelski**, D.R. Gisewhite, B.R. Williams, S.J. Nieter Burgmayer

INOR **953.** Increasing the coordination kinetics of the Acetylene Hydratase (AH) model complex via pseudo-hydroxylation. **T. Marshall**, M.A. Cranswick

INOR **954.** Mechanistic insight into nitrite to nitric oxide conversion at copper(I) and copper(II) sites. **Z. Sakhaei**, S. Kundu, J. Donnelly, T.H. Warren

INOR **955.** Extended broken symmetry approach to modeling structures and spectroscopic properties of oxidized and reduced 2Fe-2S clusters from ferredoxin. **R.A. Wheeler**, B.R. Jagger, A.M. Koval

INOR **956.** New metal complexes of tridentate N,N,O scorpionate ligands. **S.E. Sherman**

INOR **957.** Chemosensors for Ni(II) employing N/S-based donors. **E. Broering**, T.C. Harrop

INOR **958.** Synthesis and reactivity studies of nickel-selenium complexes. **L. Cordeiro**, G.P. Yap, C.G. Riordan

Section K

Moscone Center
Hall D

Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

5:30 - 7:30

INOR **959.** Transition metal complexes with triamidoborane-bridged diphosphines: Coordination chemistry, reactivity, and XAS studies. **K. Lee**, C.M. Donahue, A.V. Blake, S.R. Daly

INOR **960.** Scavenging for triiodide *via in situ* crystallization of tripalladium(II) cyclophane molecules in photo-cyclopropanation reactions. **H. Lee**, O. Jung

INOR **961.** Combined effects of peripheral fluorine and central metal on phthalocyanine properties. **R. Szlag**, M.A. Kaster, E.R. Trivedi

INOR **962.** Withdrawn.

INOR **963.** Synthesis, characterization and anticancer studies of tris-dithiocarbamato ruthenium(III) complexes. **P.A. Ajibade**

INOR **964.** Coordination complexes with guanidine-type ligands towards cleavage of aryl-heteroatom bonds found in naturally occurring feedstocks. **K.D. Feller**, B. Barry

INOR **965.** Complexes with bis-guanidine-type ligands towards insertions into sp2-heteroatom bonds. **J. Bruggen**, B. Barry

INOR **966.** Nanojar reactivity with acidic compounds and their conjugate base ligands. **C.K. Hartman**, G. Mezei

INOR **967.** Probing slow magnetic relaxation in a series of mononuclear uranium (v) compounds. **D. Lussier**, J.R. Long, D.K. Shuh

INOR **968.** Vanadium-Dependent Haloperoxidase Enzymes: A Review of Mechanism, Structure-Functional Relationships, and Coordination Environments. **K. Doucette**, C. Wallace, C.C. McLauchlan, D.C. Crans

INOR **969.** Coordination chemistry of the rhodizonate anion with Pb(II) and lanthanides: From understanding complexation to analytical applications. **J.A. Silverman**, E.V. Govor, K. Kavallieratos

INOR **970.** Theoretical computations of tunable bimetallic systems. C. Feng, M.B. Pastor, **Q. Zhao**

Section L

Moscone Center
Hall D

Lanthanide & Actinide Chemistry

A. De Bettencourt Dias, *Organizer*

5:30 - 7:30

INOR **971.** Actinide mediated C-X activation chemistry. **J.M. Dorhout**, M.J. Monreal, D.E. Morris, B. Scott, K.D. Abney, J.L. Kiplinger

INOR **972.** Very low-temperature lanthanide and actinide borates from boric acid flux. **A.T. Chemey**, S.S. Galley, T.E. Albrecht-Schmitt

INOR **973.** Gas phase chemistry of the Ln(III)-TMGA/TMTGA complexes. **X. Chen**, Q. Li, Y. Gong

INOR **974.** Design and synthesis of tri-substituted benzene compounds used as extractants in nuclear waste remediation. **B.G. Wackerle**, S.M. Biros

INOR **975.** Development of bidentate ligands containing soft donor atoms for actinide chelation. **C.C. Miller**, S.M. Biros, J.E. Bender

INOR **976.** Hyp_3Sb for separation of heavy metals. **E.G. Leach**, S.M. Biros, J.E. Bender

INOR **977.** Synthesis and characterization of (2-methoxyphenyl)diphenylphosphine derivatives for nuclear waste remediation. **E. Christoffersen**, S.M. Biros, J.E. Bender

INOR **978.** Phosphine ligands for the extraction of *f*-block elements: Use in nuclear waste remediation. **A.R. Spyker**, S.M. Biros, J.E. Bender

INOR **979.** Novel synthesis, structure, and enhanced photoluminescence of lanthanide dicyanoaurates containing aurophilic interactions. **T. Hamby**, R. Sykora, J. Hendrich, E. Kost

INOR **980.** Optimizing hydrothermal reaction conditions for lanthanide coordination polymer formation: A study of the 1,4-benzenedicarboxylate system. **J. Einkauf**, D.T. de Lill

INOR **981.** Recovery and recycling of Pu-238 in spent nuclear fuel to increase the sustainability of nuclear reactors using extraction and luminescence techniques. **M. Hudson**, G. Deblonde, R.J. Abergel, S.M. Biros

INOR **982.** Design of lanthanide half-sandwich complexes exhibiting single-molecule magnetism. **R. Khoo**, J.R. Long

Section M

Moscone Center
Hall D

Emergent Phenomena in the Solid State

B. C. Melot, E. E. Rodriguez, *Organizers*

5:30 - 7:30

INOR **983.** Structural, magnetic, and electrical properties of $Pr_2Fe_{4-x}Mn_xSb_5$ (x = 0.5, 1.0). **I.W. Oswald**, S. Li, B. Lv, J. Chan

INOR **984.** Metastable layered metal chalcogenides: From superconductivity to ferromagnetism. **B. Wilfong**, X. Zhou, H.K. Vivanco, E.E. Rodriguez

INOR **985.** Antimony nets and transition metal sublattices: The structure and properties of Ln2Fe4-xCoxSb5 (Ln = La-Pr; x <1.5). **K. Benavides**, S. Li, J.V. Burnett, B. Lv, J. Chan

INOR **986.** Evolution of the magnetic properties in the series M_2FeB_2 (M = V, Nb, Mo, Ta and W). **J. Scheifers**, V. Shukla, B. Fokwa

INOR **987.** Topochemical intercalation and ion-exchange of layered iron sulfides via low-temperature hydrothermal routes. **X. Zhou**, B. Wilfong, H.K. Vivanco, E.E. Rodriguez

INOR **988.** Effect of ionicity on magnetism of K_2MnS_2. **A. Bhutani**, P. Behera, K. Kihlstrom, M. Smylie, U. Welp, W. Kwok, E.E. Rodriguez, A. Huq, D. Shoemaker

INOR **989.** Intercalation chemistry of CoSe and $Co_{1-x}Fe_xSe$ mixed phase. **H.K. Vivanco**, B. Wilfong, X. Zhou, E.E. Rodriguez

INOR **990.** Structural design of magnetoelectric multiferroics in garnets. **A.J. Neer**, B.C. Melot

INOR **991.** Synthesis and characterization of $Hf_3Ru_{5-x}M_xB_2$ (M = Fe, Co, Ni) –towards rare-earth-free magnets. **P. Shankhari**, B. Fokwa

INOR **992.** Red, white, and blue: Controlling the luminescence of doped rare-earth oxychloride nanocrystals by ligand selection and compositional modulation. **G.V. Villalpando**, G.R. Waetzig, G.A. Horrocks, S. Banerjee

INOR **993.** Properties and design of multifunctional phyllosilicates. **E. Howard**, B.C. Melot

Section N

Moscone Center
Hall D

Chemistry is Central to Applied Materials

C. R. Bertozzi, C. J. Chang, M. A. Paley, *Organizers*

5:30 - 7:30

INOR **994.** Self-healing metallogels as the recyclable materials for selective dye adsorption and separation. **C.K. Karan**, M. Bhattacharjee

INOR **995.** Withdrawn.

INOR **996.** TAAILs - Tunable aryl-alkyl ionic liquids: A new generation of ionic liquids. **T. Strassner**

INOR **997.** Effects of calcination intensity on rutile TiO_2 white pigment production via short sulfate process. **C. Tian**

INOR **998.** Highly selective Ru/TiO_2 catalysts for HDO of phenolic compound: Effects of support structure and partial substitution of nickel for ruthenium. **S. Husremovic**, R.C. Nelson, B.G. Frederick, R.N. Austin, A. Mahdavi, S. Ki

INOR **999.** Novel approaches to the chemical syntheses of azamacrocyclic compounds and derivatives. G. Ren, E.J. Parish, Y. Lo, **H. Honda**, T. Wei

INOR **1000.** Calcium cobalt hexacyanoferrate cathodes for rechargeable divalent ion batteries. **J. Thiebes**, P. Padigi, N. Kuperman, G.M. Goncher, D. Evans, R. Solanki

INOR **1001.** Graphene-On-Silica, CMOS-integrable, thermal-guiding structures: Applications in Boolean-Logic and neuromorphic computation. **D. Loke**, J. Skelton, T. Chong, S. Elliott

‡ *Cooperative Cosponsorship*

INOR **1002.** Difluoroboron β-diketonate polylactides as luminescent oxygen sensing materials for wound imaging. **C.A. DeRosa**, S.A. Seaman, A.S. Mathew, C.M. Gorick, Z. Fan, J.N. Demas, S.M. Peirce, C. Fraser

Section O

Moscone Center
Hall D

Chemistry of Materials

C. G. Lugmair, *Organizer*

5:30 - 7:30

INOR **1003.** White light emission of lead(II) metal-organic frameworks. **A. P Peedikakkal**, J.J. Vittal

INOR **1004.** Interface-facilitated hydrothermal synthesis of large-area graphene-like carbon nanosheets from toluene. **H. Gao**, G. Wang, S. Fan, C. Dong, A. Li, X. Zhu, X. Li

INOR **1005.** Effect of electrodeposition variables on the topography and photoelectron kinetics of zinc oxide nanorods grown on graphene. C. Villarreal, **D. Pirzada**, **A. Wong**, A.K. Mulchandani

INOR **1006.** Crystal structure features and luminescent properties of the copper-doped Ca-Eu apatite. **M. Pogosova**, F. Azarmi

INOR **1007.** Structure and reducibility of CeO_2 doped with trivalent cations. **A.K. Lucid**, G.W. Watson

INOR **1008.** Facile fabrication of recyclable magnetic oxide@MOF nanocomposites for aerobic oxidation of benzylic C-H bonds. **G. Wang**, S. Fan, H. Gao, J. Wang, D. Jia

INOR **1009.** Polydopamine-induced $CaCO_3$ mineralization and its application for the synthesis of nanostructured electrocatalysts. **J. Ko**, C. Park

INOR **1010.** Molecular origins of superacidity in sulfated MOF-808. **C. Trickett**, C. Yan, T. Popp, J. Jiang, A. Huq, J.A. Reimer, M.D. Fayer, O.M. Yaghi

INOR **1011.** Polytypism in the Nowotny-Juza Compounds: Synthetic and Computational Investigation of Solution Phase I-II-V Semiconductors. **A. White**, G.J. Miller, J. Vela Becerra

INOR **1012.** Alkali bismuth dichalcogenides: Emerging energy materials for photovoltaics and thermoelectrics. **B. Rosales**, J. Vela-Becerra

INOR **1013.** $Ge_{1-x}Sn_x$/II-VI Core-shell nanostructures: Towards near IR active direct band gap semiconductors. **H. Andaraarachchi**, L. Men, J. Vela-Becerra

INOR **1014.** Withdrawn.

INOR **1015.** Cesium germanium iodide perovskite nanocrystals: Photovoltaics beyond organolead perovskites. **L. Men**, B. Rosales, N. Gentry, J. Vela-Becerra

INOR **1016.** 3D Macroporous TiO_2@CeO_2 and TiO_2@AuNP composite fabrication and application. **B. Baruah**, D. Corella, M. Geiger

INOR **1017.** Synthesis and characterization of cationic silver(I) coordination polymers for photoluminescent properties. **E. Soe**, J. Kim, S. Oliver

INOR **1018.** Organo-oxo tin cluster reactivity: Insight into cluster formation, degradation, and interconversion. **M.C. Sharps**, J.E. Hutchison, D.W. Johnson

INOR **1019.** Modelling defects in $LaMnO_3$ for solid oxide fuel cell cathodes. **A.L. Gavin**, G.W. Watson

INOR **1020.** Single molecular Wells–Dawson-like heterometallic cluster for the preparation of multifunctional carbon materials: A T1- and T2-weighted dual mode magnetic pesonance imaging agent and drug delivery system. Q. Zhang, **Y. Ling**, Y. Zhou

INOR **1021.** Two principles of reticular chemistry uncovered in a metal–organic framework of heterotritopic linkers and infinite secondary building units. **N.R. Catarineu**, A. Schoedel, P. Urban, M.B. Morla, C. Trickett, O.M. Yaghi

INOR **1022.** Novel approaches to the chemical synthesis of polycyclic electron-donor for nanoelectronic materials study. E.J. Parish, G. Ren, Y. Lo, **H. Honda**, **M. Hsiao**, T. Wei

INOR **1023.** Size tunable submicro/micro TiO_2-related spheres synthesized by sol-gel process and the applications. **Y. Chen**, K. Chan, H. Chiu, C. Lee

INOR **1024.** Integration of oriented anatase TiO_2 electron transport layer into perovskite solar cells to improve carrier separation. **H. Dehnashi**, **M.L. Mayer**, A. Yore, Y. Tran, M. Howard, A. Newaz, A.S. Ichimura

INOR **1025.** Environmentally friendly and versatile method for the synthesis of transition metal alloys and their hybrid nanoparticles. **A. Penn**, J. Sharpensteen, H.P. Rathnayake

INOR **1026.** Photoelectrochemical mechanism for instability of blue-phosphorescent Ir(III) complexes in electroluminescence devices. **S. Kim**, H. Bae, S. Park, J. Kim, J. Kim, Y. Jung, S. Sul, S. Ihn, C. Noh, S. Kim, Y. You

INOR **1027.** Fabrication and application of graphene oxide composite films. J. Shen, Y. Feng, C. Ma, D. Zhang, Z. Xiao, Z. Hui, **Y. Liu**, **Y. Min**

INOR **1028.** In situ one-pot synthetic approach towards multivariate Zr-MOFs. **Y. Sun**, H. Zhou

INOR **1029.** Hyperpolarized silicon nanoparticles as biocompatible contrast agents for ^{29}Si magnetic resonance imaging. **H. Seo**, I. Choi, D. Kim, Y. Lee

INOR **1030.** Mesoporous aluminosilicate nanoparticles hosting glow discharge plasma reduced silver nanoparticles for desulfurization of liquid hydrocarbon fuels. **J. Hauser**, D. Tran, E. Conley, J. Saunders, K. Bastillo, S. Oliver

INOR **1031.** Bottom-up synthesis approach to convert layered metal-organic framework materials into hierarchical porous structures. **Z. Li**, K. He, W. Han, K. Yeung

INOR **1032.** Discovery of earth abundant catalysts towards the implementation of a hydrogen economy. **T. Soucy**, J. Mondschein, J. McEnaney, C. Badding, R. Schaak

INOR **1033.** Preparation and structural studies of hexyldecylamine/oleic acid capped ruthenium sulfide nanocrystals. **P.A. Ajibade**

INOR **1034.** Synthesis and characterization of three cationic, isoreticular layered materials based on neodymium and α,ω-alkanedisulfonates. **A. Kareh**, S. Oliver

INOR **1035.** Selective aerobic oxidation of primary alcohols to aldehydes in functionalized mesoporous silica nanoparticles. **D. Singappuli-Arachchige**, J. Manzano, L.M. Sherman, I.I. Slowing

INOR **1036.** Crystallizing one-dimensional metal-organic sulfide as cathode material of lithium-ion battery. **Z. Ji**, C. Trickett, H. Jeong, A. Schoedel, O.M. Yaghi

INOR **1037.** Synthesis and catalytic reactions with macroporous botanically templated metal oxides and metal on carbon structures. **N. Black**, **E.G. Gillan**

INOR **1038.** Metal–organic frameworks as templates for transition metal clusters. **A. Turkiewicz**, M.I. Gonzalez, L.E. Darago, J.R. Long

INOR **1039.** Cytocompatible polysaccharide incorporated biomimetic tubules. **K. Punia**, M. Bucaro, A. Punia, A. Bykov, K.S. Raja

INOR **1040.** Efficient ammonia adsorption property of Prussian blue analogues. **A. Takahashi**, H. Tanaka, D. Parajuli, T. Nakamura, K. Minami, Y. Sugiyama, Y. Hakuta, S. Ohkoshi, T. Kawamoto

INOR **1041.** Three versatile Pt(II) oxime complexes that display anion sensing, thermochromism, and solvatochromism. **S.O. Elsiddieg**, F.R. Fronczek, A.W. Maverick

INOR **1042.** Molybdenum sulfide molecular clusters for 2D-materials. **C. Bejger**, J.L. Shott, M. Howington, J. Johnson

INOR **1043.** Crystal engineering of metal-inorganic frameworks from phosphorescent building blocks. **J. Ivy**, M.A. Omary

INOR **1044.** Nickel telluride as a bifunctional electrocatalyst for efficient water splitting in alkaline medium. **U. De Silva**, W.P. Liyanage, J. Masud, M. Nath

Section P

Moscone Center
Hall D

Inorganic Nanomaterials: Structure & Function in 0, 1 & 2 Dimensions

K. R. Kittilstved, E. J. McLaurin, *Organizers*

5:30 - 7:30

INOR **1045.** Soft-templating strategies for anisotropic Au nanomaterials and hollow multi-Au@SiO_2 nanosystems. **H. Yoo**

INOR **1046.** High performance $CsPbX_3$ perovskite quantum dot light emitting devices achieved via solid-state ligand exchange. **Y. Suh**, T. Kim, H. Park, C. Lee, J. Park

INOR **1047.** GeP_3 thin layers: Novel 2D materials revealed by first-principles calculations. **Y. Jing**

INOR **1048.** Imaging interactions between dipole emitters and single nanowires. **E. Johlin**, J. Solari, S.A. Mann, J. Wang, T. Shimizu, E. Garnett

INOR **1049.** Size control and Sb doping of solution grown two-dimensional Bi_2Se_3 nanoplates. **A.J. Bernard**, Y. Hou, D. Yu, S. Kauzlarich

INOR **1050.** Characterization of solution-based exfoliated two-dimensional nanosheets. **K. Pachuta**, A. Sehirlioglu, E. Pentzer

INOR **1051.** Vapor-Phase epitaxial growth of aligned nanowire networks of cesium lead halide perovskites ($CsPbX_3$, X = Cl, Br, I). **J. Chen**, Y. Fu, L. Samad, L. Dang, Y. Zhao, S. Shen, L. Guo, S. Jin

INOR **1052.** Pt Nanoparticle anchored molecular self-assemblies of DNA: A stable and efficient electrocatalyst for hydrogen generation. S. Anantharaj, **S. Kundu**

INOR **1053.** Titanium metal nanowires via electrospun polymer nanocomposite. **H.E. Lacy**, A.S. Ichimura, K. Teh

INOR **1054.** Solution growth of lead halide perovskite nanowires for high-performance wavelength-tunable nanowire lasers. **Y. Fu**, H. Zhu, X. Zhu, S. Jin

INOR **1055.** Polytypic phase transitions in metal intercalated 2D Bi_2Se_3 nanoribbons. **M. Wang**, K.J. Koski

INOR **1056.** Exploring biphasic routes to functionalized CdSe nanoparticles for use in solar nanocomposites. **K. Bolduc**, **M.E. Hagerman**, J.D. Kehlbeck

INOR **1057.** New route for the formation of SnSe thermoelectric materials with low thermal conductivity. **S. Kundu**, S. Yi, C. Yu

INOR **1058.** Mechanism of galvanic replacement reactions for hollow germanium nanoparticles. **X. Qi**, S. Kauzlarich

INOR **1059.** Impact of surface reconstruction on the electronic structure of PbS QD nanocrystals: Experiment and theory. **C.F. Gervasi**, H.J. Seeley, D.A. Kislitsyn, T.L. Allen, G. Nazin

INOR **1060.** Assembly of CdSe quantum dots and gold nanorods into discrete arrangements with unique optical properties. **B. Szychowski**, M. Daniel

INOR **1061.** Towards broadband-emitting 2D-perovskites LEDs. **P. Carmona Monroy**, D. Solis, E. Perez Gutierrez

INOR **1062.** Elucidating the effect of fluoride-containing ionic liquids on indium phosphide nanocrystals. **S. Lee**, E.J. McLaurin

Section Q

Moscone Center
Hall D

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

5:30 - 7:30

INOR **1063.** Large-scale synthesis of Sb_2Q_3 (Q = S, Se) nanofibers topotactically converted from ternary metal chalcogenides and their optical and transport properties. **H. Lee**, M. Kim, B. Yoo, K. Ahn, I. Chung

INOR **1064.** Hydrothermal synthesis and characterization of three-dimensional titanium(III) phosphites. **L. Hung**, S. Wang

INOR **1065.** Mechanoconglomeration and mechanoracemization of gold(I) complex crystals with optical properties alternation. **M. Jin**, T. Seki, H. Ito

INOR **1066.** Synthesis, crystal structure, and thermoelectric properties of new phosphides $BaCu_5P_3$ and $Ba_4Cu_{11.2}Mg_{2.8}P_{10}$. **J. Mazzetti**, J. Wang, K. Kovnir

INOR **1067.** Synthesis and structural evaluation of manganese doped cobalt oxides. **A.R. Thuli**, A.M. Morey

INOR **1068.** Sol-gel synthesis and characterization of lithium nickel cobalt oxides. **J.J. McCune**, A.M. Morey

INOR **1069.** Heat treatment intensity on rutile pigment production from unenriched industrial TiOSO4 solution via short sulfate process. **C. Tian**

INOR **1070.** Two zinc titanophosphates containing organic linkers from in situ metal/ligand reactions. L. Huang, P. Chen, L. Hung, **S. Wang**

INOR **1071.** Superhard alloys of transition metal dodecaborides: $Zr_{1-x}Y_xB_{12}$, $Zr_{1-x}Sc_xB_{12}$ and $Y_{1-x}Sc_xB_{12}$. **G. Akopov**, M.T. Yeung, Z.C. Sobell, C.L. Turner, R.B. Kaner

INOR **1072.** Metal flux and supercritical fluid syntheses of actinide materials. **W. Potter**, T.E. Albrecht-Schmitt, S.E. Latturner

INOR **1073.** Optimization of the CsCl reduction-oxidation flux synthesis of Cs-Zn-Sb clathrates. **S. Heinrich**, B. Owens-Baird, J. Dolyniuk, K. Kovnir

INOR **1074.** Thermoelectric properties of n-type SnSe-based materials. **J. Cha**, K. Ahn, I. Chung

INOR **1075.** Tunable optical properties of Sn-based perovskite compounds. **M. Lee**, I. Chung

INOR **1076.** Novel light emitting phosphors based on olivine structure type oxide, $CaYGaO_4$. **S.M. Araiza**, K. Slowinska, S. Derakhshan

INOR **1077.** Chemical conjugation of rare-earth oxychloride nanocrystals to hybrid organic-inorganic perovskite nanoplatelets for solid-state lighting applications. **F.A. Rodriguez Ortiz**

INOR **1078.** Stabilization of GdB_{12} in $Zr_{1-x}Gd_xB_{12}$ under ambient pressure. G. Akopov, **Z. Sobell**, M. Yeung, R.B. Kaner

INOR **1079.** Using a dataset of magnetic material properties to screen for magnetocalorics. **J.D. Bocarsly**, E. Levin, S. Wilson, R. Seshadri

INOR **1080.** Effects of microstructurally induced strain on magnetic properties of biphasic Heusler systems. **E. Levin**, M. Buffon, P. Callahan, J. Stinville, S. Mooraj, D. Gianola, T. Pollock, R. Seshadri

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

WEDNESDAY MORNING

Section A

Moscone Center
2009

Deposition & Etching of Nanostructures

Cosponsored by COLL‡

Financially supported by ACS Publications, Strem Chemical

H. Fairbrother, A. V. Walker, *Organizers*

L. McElwee-White, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 INOR **1081.** Using inherent substrate-dependent nucleation to promote selective-area atomic layer deposition. **G. Parsons**, P. Lemaire, M. Ritz, C.J. Oldham

9:10 INOR **1082.** Deposition of ZnO nanostructures on graphene: Application as tin oxide-free photoanodes. **C. Villarreal**, D. Pirzada, A. Wong, A.K. Mulchandani

9:35 INOR **1083.** Sustainable manufacturing of functional materials. **C.J. Carmalt**

10:10 Intermission.

10:30 INOR **1084.** Cobalt metal thin films: Precursor syntheses, atomic layer deposition, and selective growth. **C.H. Winter**

11:05 INOR **1085.** Chemical self-assembly strategies for metal-organic surface structures. J. Kestell, R. Abuflaha, D. Olson, **W.T. Tysoe**

11:30 INOR **1086.** New precursor chemistries for ALD of transition metal oxides. **A. Devi**

Section B

Moscone Center
2011

Celebrating 60 Years of the Division of Inorganic Chemistry

Young Investigators & Officers

D. C. Crans, *Organizer*

M. J. Clarke, *Organizer, Presiding*

L. M. Berreau, C. Turro, *Presiding*

8:00 Introductory Remarks.

8:05 INOR **1087.** Chemical tools for investigating cellular zinc metalloenzymes. **E.L. Que**

8:35 INOR **1088.** Engineering molecular materials for applications in energy storage. A. Baumann, D. Burns, **V. Thoi**

9:05 INOR **1089.** Nonaromatic tetrapyrrole metal complexes supporting a multielectron redox chemistry for efficent dioxygen activation. **J. Rosenthal**, J. Eddy, T. Qiu

9:35 INOR **1090.** De novo design of metalloproteins. **I.V. Korendovych**

10:05 Intermission.

10:20 INOR **1091.** Highly stable Metal-organic frameworks with ultrahigh capacitance. **D. Feng**, Z. Bao

10:50 INOR **1092.** Coordination chemistry with fullerene-based ligands. **A.L. Balch**, M.M. Olmstead, A. Aghabali, S. Jun

11:20 INOR **1093.** Employing novel porphyrinoid ligands to access biomimetic manganese and iron complexes of relevance to O_2-activating heme enzymes. **D.P. Goldberg**, J. Zaragoza, R.A. Baglia, J. Sacramento

11:50 INOR **1094.** Lanthanide complexes and materials with sensitized metal-centered luminescence. **A. De Bettencourt Dias**

Section C

Moscone Center
2016

Frontiers in Heavy Element Electronic Structure

Cosponsored by NUCL

D. L. Clark, D. K. Shuh, *Organizers*

L. Soderholm, *Organizer, Presiding*

8:30 INOR **1095.** Up all night with Bruce: From computations to experiments to real computations & experiments. **G.G. Stanley**

8:50 INOR **1096.** Designing activated carbons for Hg removal from coal combustion flue gas. **R. Cayton**

9:10 INOR **1097.** Counting electrons: What they don't teach you in general chemistry. **J.S. D'Acchioli**, M.K. Heili, P. Sit, E.D. Speetzen, A. Webster, C. Mueller, D. Cunningham

9:30 INOR **1098.** Electronic structure and metal-metal bonding in heterobimetallic and heterotrimetallic complexes of a redox-active metalloligand. **A.F. Heyduk**, M. Wojnar, K.E. Rosenkoetter

9:50 INOR **1099.** Bonding with Bruce. **D.L. Clark**

10:10 Intermission.

10:30 INOR **1100.** Intriguing aspects of non-innocent ligandsin transition metal complexes. **M.B. Hall**

10:50 INOR **1101.** Give It some thought: Inorganic chemistry and nanotechnology. **C.J. Murphy**

11:10 INOR **1102.** Magnetic circular dichrosim and electronic absorption spectra of multiply metal-metal bonded rhenium dimers. **A.P. Sattelberger**, M.L. Kirk, F. Poineau, E. Johnstone, K. Czerwinski, D. Habel-Rodriguez

11:30 INOR **1103.** Heavy element chemistry in a heterogeneous context. **W.F. Schneider**

11:50 INOR **1104.** Excited states of mononuclear and dinuclear complexes and their applications. **C. Turro**

Section D

Moscone Center
2018

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

S. E. Latturner, F. Rabuffetti, *Presiding*

8:30 INOR **1105.** Lead- and tin-based two-dimensional hybrid organic-inorganic iodide perovskites: Structure, properties and application in planar solar cells. **L. Mao**, H. Tsai, W. Nie, L. Ma, J. Im, C. Stoumpos, C. Malliakas, M.R. Wasielewski, A.D. Mohite, M.G. Kanatzidis

8:45 INOR **1106.** Pressure-induced structural, electronic, and optical evolution of hybrid perovskites. **A. Jaffe**, Y. Lin, C. Beavers, J. Voss, W. Mao, H. Karunadasa

9:00 INOR **1107.** Tuning indirect to direct bandgaps in double perovskites. **T. Tran**, J. Panella, J. Chamorro, J.R. Morey, T. McQueen

9:15 INOR **1108.** Structure and dynamics of perovskite formamidinium lead iodide: Phase transitions, reentrant properties, persistent molecular motion, and large positive thermal expansion. **D.H. Fabini**, G. Laurita-Plankis, C. Stoumpos, T. Siaw, S. Han, M.G. Kanatzidis, R. Seshadri

9:30 INOR **1109.** Trends in the lone pair-induced local off-centering of tin and lead atoms in halide perovskites. **G. Laurita-Plankis**, D.H. Fabini, C. Stoumpos, M.G. Kanatzidis, R. Seshadri

9:45 INOR **1110.** Negative thermal expansion and other anomalous properties in mixed metal fluorides with structures related to that of ReO_3: A perovskite with helium on the A-site? **A.P. Wilkinson**, B. Hester

10:00 INOR **1111.** Tuning photochemical and photophysical properties of metallosupramolecular materials. **A. Razgoniaev**, A. Ostrowski

10:15 Intermission.

10:30 INOR **1112.** Synthesis of new complex metal hydrides and carbides from ytterbium/lithium flux. M. Dickman, **S.E. Latturner**

10:45 INOR **1113.** *In situ* identification of kinetic factors that expedite inorganic crystal formation and discovery. **Z. Jiang**, A. Ramanathan, D. Shoemaker

11:00 INOR **1114.** Dynamic origins of noncentrosymmetry in $KNaNbOF_5$. **M. Holland**, **K.R. Poeppelmeier**, J. Rondinelli, N. Charles

11:15 INOR **1115.** In-situ reduction study of the effect of anion concentration in the Fe-Ga-S system. **R. McAuliffe**, D. Shoemaker

11:30 INOR **1116.** Design of piezoelectric heterostructural alloys. **S. Miller**, K. Talley, A.W. Weimer, A. Zakutayev, S. Lany, C. Musgrave, G. Brennecka, A. Holder

11:45 INOR **1117.** Piezoelectrics: Putting the squeeze on new materials. **M. Dolgos**

12:00 INOR **1118.** Low-Barrier "H-M-H" molecular rotor. **E. Prack**, C.A. O'Keefe, J.K. Moore, A. Lai, A.J. Lough, P.M. Macdonald, M.S. Conradi, R.W. Schurko, U.W. Fekl

12:15 INOR **1119.** Synthesis of bimetallic trifluoroacetates through a crystallochemical investigation of their monometallic counterparts: The case of $(A, A')(CF_3COO)_2.nH_2O$ (A, A' = Mg, Ca, Sr, Ba, Mn). B. Dhanapala, N. Mannino, K. Dissanayake, L. Suescun, **F. Rabuffetti**

Section E

Moscone Center
2020

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

B. E. Cohen, F. Rabuffetti, *Presiding*

8:00 INOR **1120.** Pnictide precursors for pnictide-based thermoelectric nanomaterials. **A. Das**

8:20 INOR **1121.** Syntheses of $Zn_{1-x}Cd_xS$ nanocrystals with tunable band structure for efficient reduction of nitroaromatics in water. **M. Kaur**

8:40 INOR **1122.** Improved covalent protein labeling and single-molecule optical properties of compact CdSe/CdS quantum dots. **B.E. Cohen**, A. Powers, S. Wichner, A. Yildiz

‡ *Cooperative Cosponsorship*

9:00 INOR **1123.** Investigations of using environmentally responsive polymers as capping materials for aluminum nanoparticles. **W. Zeng**, S.W. Buckner, P.A. Jelliss

9:20 INOR **1124.** Ultrathin copper based core shell nanowires for high-performance transparent conductors - from synthesis to application. **F. Cui**, P. Yang, L. Dou, Z. Niu, Y. Yu

9:40 INOR **1125.** Chemically and structurally flexible hosts for Yb-Er sensitizer-activator pairs. K. Dissanayake, B. Dhanapala, **F. Rabuffetti**

10:00 Intermission.

10:15 INOR **1126.** Flexible transparent film heaters based on random networks of silver nanowires: Synthesis, characterization and integration into devices. **C. Celle**, T. Sannicolo, D. Toybou, A. Cabos, J. Simonato

10:35 INOR **1127.** Fabrication of high quality compressible 3D graphene aerogel based on graphene oxide nanobelts and for supercapacitor. T. Fan, Z. Xiao, T. He, Y. Liu, **Y. Min**

10:55 INOR **1128.** Expansion of the family of gigantic palladium macrocycles based on {Pd84}. **L. Cronin**

11:15 INOR **1129.** Spatially orthogonal chemical functionalization of a hierarchical pore network for catalytic cascade reactions. **C.M. Parlett**, S.K. Beaumont, L.J. Durndell, M. Isaacs, N.S. Hondow, K. Wilson, A.F. Lee

11:35 INOR **1130.** Synthesis and characterization aluminum nanoparticles capped by polymerization of acrylic monomers. **C.O. Nyapete**, P.A. Jelliss, S.W. Buckner

11:55 INOR **1131.** Synthesis and characterization of *o*-carborane passivated aluminum nanoparticles. **A. Benziger**, S.W. Buckner, P.A. Jelliss

Section F

Moscone Center

2022

Lanthanide & Actinide Chemistry

Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

R. J. Abergel, K. Kavallieratos, D. A. Penchoff, *Presiding*

8:30 INOR **1132.** Terminal Uranium(IV) sulfido and hydrosulfido complexes: Theoretical study of the uranium-sulfur bond. **C. Alvarez Lamsfus**, L. Maron

8:50 INOR **1133.** Selective separation of americium from europium using 2,9-bis(triazine)-1,10-phenanthrolines in ionic liquids: A new twist on an old story. **N.J. Williams**, J. Dehaudt, C.W. Abney, H. Luo, S. Dai

9:10 INOR **1134.** Computational prediction of paramagnetic NMR spectra of f-element complexes. **H. Moylan**, J. McDouall

9:30 INOR **1135.** Thermochemical and structural predictions of lanthanide- and actinide-containing compounds: A computational perspective. **D.A. Penchoff**, C. Peterson, A.K. Wilson

9:50 Intermission.

10:00 INOR **1136.** Actinide coordination with bio-inspired ligands: A bridge between fundamental f-element chemistry and new therapeutic drug development. **R.J. Abergel**, G. Deblonde, I. Captain, P. Agbo, A. Ricano, D. An

10:20 INOR **1137.** Controlled synthesis of lanthanide nanomaterials with covalent organic frameworks. **A. Braun**, S. Alayoglu, C. Booth, D. Olive, M. Straub, S.G. Minasian

10:40 INOR **1138.** Trivalent f-metal coordination and extraction by tripodal sulfonamide ligands and analogs. E.V. Govor, V.A. Anagnostopoulos, A.N. Morozov, A.M. Mebel, R.G. Raptis, **K. Kavallieratos**

11:00 Intermission.

11:10 INOR **1139.** Synthesis and redox non-innocent reactivity of bis(NHC)borate-supported thorium complexes. **M. Garner**, S. Hohloch, L. Maron, J. Arnold

11:30 INOR **1140.** Exploring water selective properties and uptake rates of a uranium metal-organic nanotube. **A.S. Jayasinghe**, M. Payne, D. Unruh, T. Forbes

11:50 INOR **1141.** Chalcogenide insertion reactivity of a thorium-alkyl complex supported by amidinate ligands. **N. Settineri**, J. Arnold

Section G

Moscone Center

2024

Nanoscience

B. G. Trewyn, *Organizer*

B. A. Hernandez-Sanchez, *Presiding*

8:00 INOR **1142.** Hyaluronic acid conjugated carbon quantum dots for bioimaging and targeted drug delivery in ophthalmology. **B.B. Karakocak**, J. Liang, P. Biswas, N. Ravi

8:20 INOR **1143.** Bacteriophage-conjugated quantum dots as *in vivo* luminescent bioimaging agents. **W.C. Corbin**, M. Casillas, J. Pelowitz, C. Ashley, B.A. Hernandez-Sanchez

8:40 INOR **1144.** Bioconjugation chemistry in luminescent gold nanoparticles. **R. Vinluan**, J. Zheng

9:00 INOR **1145.** Nanoelectronic signaling approaches for chemical sensing and fundamental investigation of chemical/biological systems. **M. Ding**, Y. Huang, X. Duan

9:20 INOR **1146.** Magnetically stimulated release from Medusa particles. B.J. McCormick, M.E. Whitaker, E. Roedern, K. O'Connor, R.R. Shah, S. Pan, J.A. Nikles, C.S. Brazel, **D.E. Nikles**

9:40 INOR **1147.** Liquid biopsy for detecting ductal pancreatic adenocarcinoma. **S.H. Bossmann**, H. Wang, M. Kalubowilage, O. Covarrubias Zambrano, A.P. Malalasekera, A.S. Yapa, R. Ortega, Y. Toledo, A. Kasi, S. Williamson, C.T. Culbertson, D.L. Troyer

10:00 Intermission.

10:10 INOR **1148.** Synthesis of multifunctional dendronized-gold nanoparticles for bimodal in vivo imaging. **A. Saha Ray**, M.W. Brechbiel, M. Daniel

10:30 INOR **1149.** Developing lanthanide doped alkaline earth chalcogenide nanoparticles for scintillators and bioimaging agents. **B.A. Hernandez-Sanchez**, T.J. Boyle, T.N. Lambert, P. Lu

10:50 INOR **1150.** Light scattering study on the interaction of poly(N-isopropylacrylamide) and transition metal dications. **L. Fulton**, J. Tsavalas, W.R. Seitz, R.P. Planalp

11:10 INOR **1151.** Atomically precise Organomimetic Cluster Nanomolecules (OCNs). **E.A. Qian**, A.I. Wixtrom, J.C. Axtell, A. Saebi, D. Jung, P. Rehak, Y. Han, E. Hakim Moully, D. Mosallaei, S. Chow, M. Messina, J. Wang, A.T. Royappa, A.L. Rheingold, H.D. Maynard, P. Kral, A.M. Spokoyny

11:30 INOR **1152.** Bottom-up synthesis and self-assembly of atomically precise pristine and nitrogen-doped graphene nanoribbons. **A. Sinitskii**

11:50 INOR **1153.** Integrating sphere microscopy to quantify losses and limits in nanoscale solar cells. **S.A. Mann**, S. Oener, A. Cavali, J. Haverkort, E. Bakkers, E. Garnett

12:10 INOR **1154.** Approaching the hole mobility limit of GaSb nanowires. Z. Yang, **J.C. Ho**

Section H

Moscone Center

3000

Organometallic Chemistry: Applications to Organic Transformations

N. S. Radu, *Organizer*

B. Fraga, *Presiding*

8:30 INOR **1155.** Mechanistic understanding of catalyst-controlled and tunable, chemoselective silver-catalyzed intermolecular nitrene transfers. **T. Yang**, J.F. Berry

8:50 INOR **1156.** Preparation and characterization of copper(I) diazabutadiene complexes and catalytic applications. **B. Zelenay**, F. Maseras, S. Diez-Gonzalez

9:10 INOR **1157.** Synthesis and reactivity of weakly interacting dicopper systems. M.B. Pastor, T. Betley, **Q. Zhao**

9:30 INOR **1158.** Synthesis and reactivity of mixed-ligand dirhodium(II) complexes with pendant axial ligands. **A. Darko**, D. Cressy, B. Anderson, W.A. Sheffield

9:50 INOR **1159.** Selective *ortho* C-H activation of pyridines directed by Lewis acidic boron of PBP pincer iridium complexes. **W. Shih**, O. Ozerov

10:10 INOR **1160.** Mechanistic insight into carbon-sulfur bond formation at cobalt (III). **B.J. Foley**, C. Palit, O. Ozerov

10:30 INOR **1161.** Oxidative reactivity of organometallic Ni^{II}, Ni^{III} & Ni^{IV} complexes in the formation of C-C bonds. **M.B. Watson**, L.M. Mirica

10:50 INOR **1162.** Mechanistic study of an improved nickel precatalyst for the Suzuki-Miyaura reaction of aryl sulfamates: Understanding the role of nickel(I) species. **M. Mohadjer Beromi**, N. Hazari

11:10 INOR **1163.** Rational design of improved Pd(II) precatalysts and their application towards new cross-coupling reactions. P. Melvin, **N. Hazari**

11:30 INOR **1164.** Mechanistic investigations of palladium(II) precatalysts: Effects of reaction conditions on precatalyst activity in the Suzuki cross-coupling of aryl bromides. **K.L. Barnett**, K.H. Shaughnessy

11:50 INOR **1165.** Half-sandwich ruthenium catalysts with enantiopure primary amine-tethered N-heterocyclic carbenes for asymmetric ketone hydrogenation. **K. Wan**, M.M. Sung, A.J. Lough, R.H. Morris

12:10 INOR **1166.** Asymmetric transfer hydrogenation of ketones by rhodium and iridium complexes of chiral oxazolidine fused N-heterocyclic carbene ligands. B. Ramasamy, **P. Ghosh**

Section I

Moscone Center

3010

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Polymerization, Coordination Chemistry & Interfacial Catalysis

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREM, Argonne National Lab, Northwestern University

A. Facchetti, T. Lohr, *Organizers*

M. Delferro, *Presiding*

8:30 Introductory Remarks.

8:35 INOR **1167.** Controlling ethylene/α-olefin selectivity with molecular olefin polymerizaiton catalysts. **J. Klosin**

9:05 INOR **1168.** Performance polymers in the petroleum additives industry. **N.A. Cain**, J.D. Moore

9:35 INOR **1169.** Deactivation and reactivation of methylaluminoxane (MAO) and the derived metallocene catalysts. New insight into MAO active site structure and activation mechanism. **L. Luo**, A. Jain, J. Harlan

10:05 INOR **1170.** Recent developments concerning post-metallocene olefin poly/oligomerization catalysts at Mitsui Chemicals. **M. Kondo**, S. Ishii, N. Uehara, Y. Tanaka, K. Michiue, K. Tanaka

10:35 Intermission.

10:45 INOR **1171.** Can microdroplets catalyze chemical reactions? **R.N. Zare**

11:15 INOR **1172.** Reactions of C-Au and C-H bonds with polynuclear metal carbonyl cluster complexes. **R.D. Adams**, P. Dhull, V. Rassolov, J. Tedder, Y. Wong

11:45 INOR **1173.** Sustainable polymers with complete recyclability for a circular economy. **E.Y. Chen**

Section J

Moscone Center

3012

Chemistry is Central to Applied Materials

Cosponsored by MPPG‡

C. J. Chang, *Organizer*

C. R. Bertozzi, M. A. Paley, *Organizers*, *Presiding*

8:30 INOR **1174.** Hybrid perovskites under pressure: Accessing new properties through lattice compression. A. Jaffe, Y. Lin, D. Umeyama, C. Beavers, J. Voss, W. Mao, **H. Karunadasa**

9:05 INOR **1175.** Densely-functionalized porous polymers for ammonia capture, metal ion separations, and battery applications. G. Barin, S. Demir, J.C. Axelson, M. Aubrey, J.A. Mason, N. Brune, M.K. Taylor, S. Lee, J. Van Humbeck, D.K. Shuh, C.J. Chang, **J.R. Long**

9:40 INOR **1176.** Withdrawn.

10:15 Intermission.

10:30 INOR **1177.** Electrolyte-Mediated assembly of charged nanoparticles. **M. Olvera De La Cruz**

11:05 INOR **1178.** Seaweed-Based synthesis of nanostructures for multiple energy storage. **D. Yang**, X. Yao

11:40 INOR **1179.** Framework chemistry and its global reach. **O.M. Yaghi**

Section K

Moscone Center
3001

Switchable Catalysts

J. A. Byers, *Organizer*

P. Diaconescu, *Organizer, Presiding*

F. Breher, *Presiding*

8:30 INOR **1180.** Altering the selectivity of iron-catalyzed hydrocarbon upgrading. **P.J. Chirik**, J. Steves, V. Schmidt

9:00 INOR **1181.** Reversible interconversion of CO_2/H_2 and formic acid using Cp*Ir(III) complexes with proton responsive ligands. **E. Fujita**, J.T. Muckerman, Y. Himeda

9:30 INOR **1182.** Switchable polynuclear complexes consisting of ambidentate ligands. **F. Breher**

10:00 INOR **1183.** Redox catalysis for biomass degradation. **C. Stephenson**

10:30 Intermission.

10:45 INOR **1184.** Cerium clusters supported by trimetallic crown ethers as catalysts for alternative copolymerization of cyclohexene oxide and CO_2. **K. Mashima**, H. Nagae, R. Aoki, T.P. Spaniol, J. Okuda

11:15 INOR **1185.** One-pot switchable catalytic processes involving the copolymerization of epoxides and carbon dioxide. **D.J. Darensbourg**

11:45 INOR **1186.** Supramolecular approach to enzyme mimics. **C.A. Mirkin**

12:15 Concluding Remarks.

Section L

Moscone Center
3003

Bioinorganic Chemistry

S. A. Koch, *Organizer*

D. Wang, Y. Zhang, *Presiding*

8:30 INOR **1187.** Study the interactions of biometals with microtubule binding domain of tau protein, contribution to Alzheimer's diseases. **S. Ahmadi**, S. Zhu, R. Sharma, R. Dutta Majumdar, R. Soong, D. Wilson, A. Simpson, H. Kraatz

8:50 INOR **1188.** Small biomolecules reactions with carbon disulfide: Pursuing a primary biological target. **M.L. Souza**, A. DeMartino, P.C. Ford

9:10 INOR **1189.** Biomimetic, catalytic water oxidation by molecular nickel complexes with redox active ligands. **D. Wang**, C. Bruner

9:30 INOR **1190.** Withdrawn.

9:50 INOR **1191.** Can $Fe^{IV}(O)$'s swim? The aqueous chemistry of the $[Fe^{IV}(O)(TMC)]^{2+}$ complex. **J. Klein**, A. Shokri, A. Draksharapu, J. Prakash, C.J. Cramer, L. Que

10:10 Intermission.

10:20 INOR **1192.** Proton management within a [FeFe] hydrogenase model complex. **K. Chu**, M. Chiang, Y. Liu

10:40 INOR **1193.** HNO Binding in heme proteins: Effects of iron oxidation state, axial ligand, and protein environment. R. Khade, Y. Yang, Y. Shi, **Y. Zhang**

11:00 INOR **1194.** FerricCEST: A low-spin Fe(III) complex as paraCEST MRI contrast agent. **P.B. Tsitovich**, J.R. Morrow

11:20 INOR **1195.** Photoreleasing caged molecules containing nitrile functionality from Ru(II) complexes of the bulky 6-phenyl-2,2'-bipyridine ligand. **S. Saha**, R. Coll, K.L. Fillman, J. Pellois, C. Turro, K.R. Dunbar

11:40 INOR **1196.** Typel/TypeII dual photoreactivity of new promising Ru-polypiridyl thiophene complexes: A theoretical exploration. **M. Alberto**, J. Pirillo, N. Russo, C. Adamo

12:00 INOR **1197.** Dual targeting redox-active gold(I) N-Heterocyclic carbene complexes: A new approach to cancer treatment. **K. Arumugam**, M. Miles, R. McCall, J. Arambula

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Sponsored by PHYS, Cosponsored by INOR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Spectroscopy & Microscopy of Photocatalytic & PEC Materials

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

WEDNESDAY AFTERNOON

Section A

Moscone Center
2009

Deposition & Etching of Nanostructures

Cosponsored by COLL‡

Financially supported by ACS Publications, Strem Chemical

H. Fairbrother, A. V. Walker, *Organizers*

L. McElwee-White, *Organizer, Presiding*

1:30 INOR **1198.** Experimental and computational development of single source precursors to tin-doped germanium nanocrystals. **J. Vela-Becerra**

2:05 INOR **1199.** Surface chemistry guided nanoparticle deposition in plasmonic hotspots. **J. Millstone**

2:40 INOR **1200.** Mechanism based design of precursors for FEBID. **L. McElwee-White**

3:15 Intermission.

3:35 INOR **1201.** Nanosoldering carbon nanotube junctions with metal via local chemical vapor deposition for improved device performance. J. Do, D. Estrada, X. Xie, N. Chang, J.A. Rogers, E. Pop, J. Lyding, **G.S. Girolami**

4:10 INOR **1202.** Designing high-performance nanoscale catalysts for small molecule reactions: Probing size and composition-dependent electrocatalytic behavior in noble metal-based nanowires. **S.S. Wong**

4:45 INOR **1203.** Lanthanide oxides and lanthanide nitrides via vapor phase approaches. **H. Parala**

Section B

Moscone Center
2011

Celebrating 60 Years of the Division of Inorganic Chemistry

Members

D. C. Crans, *Organizer*

M. J. Clarke, *Organizer, Presiding*

A. De Bettencourt Dias, P. K. Dorhout, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **1204.** Meanderings in atom transfer reaction chemistry, structure, electronic structure and thermochemistry. **J.M. Mayer**

2:05 INOR **1205.** Tuning transition metal redox potentials through the incorporation of redox-inactive cations: A route to breaking potential dependent scaling relationships? A.H. Reath, T. Chantarojsiri, **J.Y. Yang**

2:35 INOR **1206.** Understanding the formation of Pd(I) and Ni(I) complexes in cross-coupling reactions. **N. Hazari**

3:05 Intermission.

3:20 INOR **1207.** Interplay of inorganic and organic chemistry in catalyst design and performance. **D.B. Grotjahn**

3:50 INOR **1208.** Evaluating the cluster-surface analogy with electronically and geometrically flexible macrocyclic ligands. P. Cui, Q. Wang, B. Manor, P. Carroll, **N.C. Tomson**

4:20 INOR **1209.** Carbon dioxide reduction with transition metal catalysts composed of pyridines and N-heterocyclic carbenes based chelates. **D.B. Burks**, S. Siek, C. Boudreaux, J.H. Delcamp, E.T. Papish

4:40 INOR **1210.** Controlling reactivity of small molecules through confinement. M.D. Johnson, **D.C. Crans**

5:10 Concluding Remarks.

Section C

Moscone Center
2016

Frontiers in Heavy Element Electronic Structure

Cosponsored by NUCL

D. K. Shuh, L. Soderholm, *Organizers*

D. L. Clark, *Organizer, Presiding*

1:30 INOR **1211.** From a high-valent iron nitride to a low-valent pentad of iron nitrosyl complexes $\{FeNO\}^{6\text{-}10}$ stabilized by a chelating, N-anchored tris-*N*-heterocyclic carbene ligand. **K. Meyer**

1:50 INOR **1212.** Design and properties of photoredox chromophores that are stronger reductants than alkali metals. **M.D. Hopkins**, H.B. Vibbert

2:10 INOR **1213.** Evaluating the electronic structure of LnII(C5H4SiMe3)31- complexes. **S.A. Kozimor**, E.R. Batista, J.W. Engle, W.J. Evans, M.G. Ferrier, M. Fieser, J. Pacheco, A. Olson, J. Su, T. Vitova, P. Yang

2:30 INOR **1214.** Chemistry of iron complexes toward the synthesis of FeX multiple bonds. **P.T. Wolczanski**, B. Jacobs, S.N. MacMillan, T.R. Cundari

2:50 INOR **1215.** Actinides, f-orbitals, and multiple bonds: These are just a few of Bruce's favorite things. **J.L. Kiplinger**

3:10 Intermission.

3:30 INOR **1216.** Addition of H-X to Mn and Ru amide bonds: Catalysts for formic acid decomposition and the aldehyde water shift reaction. **J.M. Boncella**, A.M. Tondreau, N.H. Anderson, B. Scott

3:50 INOR **1217.** New thoughts on the speciation of polychalcogenides in solutions: From lapis lazuli, to the paper industry, to synthetic inorganic chemistry and why my clothes smell so bad. **P.K. Dorhout**

4:10 INOR **1218.** Recent advances in the chemistry of tris(cyclopentadienyl) rare-earth and actinide metal complexes. **W.J. Evans**

4:30 INOR **1219.** Betwixt or between? Inter- and intraligand redox processes in Fe and Co-SNS coordination complexes. **R. Baker**

4:50 INOR **1220.** Formation of C(sp3)-N bonds from Rh^{III}-Me and Ir^{III}-Et complexes. T. Stevens, T.R. Cundari, **K.I. Goldberg**

Section D

Moscone Center
2018

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

A. F. Cozzolino, *Presiding*

1:30 INOR **1221.** Water dynamics in three-dimensional extended lead(II) structures: Multiple single-crystal-to-single-crystal transformations. **R.A. Burrow**, B. Brummelhaus de Menezes

1:50 INOR **1222.** Withdrawn.

2:10 INOR **1223.** Structural characteriation of framework–guest interactions in metal–organic frameworks. **M.I. Gonzalez**, R.L. Siegelman, E.D. Bloch, J.A. Mason, M. Kapelewski, W. Queen, S.J. Teat, K.J. Gagnon, J.R. Long

2:30 INOR **1224.** Confinement of inorganic clusters in metal–organic frameworks with coordinating sites. **M.I. Gonzalez**, A. Turkiewicz, L.E. Darago, J.R. Long

2:50 INOR **1225.** Tuning the adsorption-induced phase change in the flexible metal-organic framework Co(bdp). **M.K. Taylor**, J.R. Long

3:10 Intermission.

3:25 INOR **1226.** Pyrazolate-based porphyrinic MOFs with extraordinary stability and catalytic activity for C–H bond halogenation. **K. Wang**, H. Zhou

3:45 INOR **1227.** Porphyrin-based metal organic frameworks for electrocatalysis. **A. Fateeva**, F. Maillard, B. Abeykoon, J. Tommasino

4:05 INOR **1228.** Metal-organic layers for earth-abundant metal catalysis. **Z. Lin**, W. Lin, T. Sawano, N.C. Thacker, C. Wang

4:25 INOR **1229.** Metal-organic frameworks nodes for earth-abundant metal catalysis. **P. Ji**, K. Manna, Z. Lin, W. Lin

4:45 INOR **1230.** Incorporating p-block catalysts into robust metal organic frameworks. P. Larson, B. Tahmouresilerd, J. Cheney, **A.F. Cozzolino**

‡ *Cooperative Cosponsorship*

5:05 INOR **1231.** Metal-Organic frameworks with tunable bandgap. **J. Park**, D. Feng, Z. Bao

Section E

Moscone Center

2020

Inorganic Spectroscopy

V. C. Popescu, *Organizer, Presiding*

1:30 INOR **1232.** Achieving surface sensitivity in soft x-ray spectroscopy: Transient reflectivity of charge transfer dynamics in iron oxide. **A. Cirri**, J. Husek, S. Biswas, L. Baker

1:50 INOR **1233.** Probing molecular magnetism with neutron scattering. **S. Stavretis**, D.H. Moseley, A.A. Podlesnyak, C.M. Brown, Y. Cheng, L.L. Daemen, A.J. Ramirez-Cuesta, X. Wang, C.M. Hoffmann, S.O. Diallo, Z. Zhu, M. Guo, J. Tang, H. Cui, F. Fei, X. Chen, Z. Xue

2:10 INOR **1234.** Design principles for porous materials containing quantum sensors. **J. Zadrozny**, A. Gallagher, D. Harris, D.E. Freedman

2:30 INOR **1235.** Probing ion-pairing trends in aqueous polyoxometalate solutions. **D. Sures**, K. Kozma, P.I. Molina, S. Serapian, C. Bo, M.D. Nyman

2:50 INOR **1236.** High-valent states in cobalt cubanes and clusters: Relevance to O–O bond formation. **R.G. Hadt**, C. Brodsky, D. Hayes, L.X. Chen, D.G. Nocera

3:10 INOR **1237.** Studies of single-molecule magnets by far-IR and Raman in magnetic fields. **D.H. Moseley**, S. Stavretis, K. Thirunavukkuarasu, Q. Chen, H. Zhou, J. Ludwig, D. Smirnov, Z. Zhu, M. Guo, J. Tang, F. Fei, H. Cui, X. Chen, Z. Xue

3:30 INOR **1238.** Capturing intermediates of molecular solar fuels catalysts by time-resolved mid-IR spectroscopy. **L. Hammarstrom**, R. Lomoth, S. Ott

3:50 INOR **1239.** Light driven activation of O_2 with iron(II) polypyridyl complexes. **J. Chen**, A. Draksharapu, W.R. Browne

4:10 INOR **1240.** Relativistic effects on the spectra and redox properties of 5d metallocorroles. **A. Ghosh**, **R.F. Einrem**, A. Alemayehu

4:30 INOR **1241.** Systematic study of luminescence rigidochromism on ambipolar polyimine rhenium(I) complexes. **G.A. Salazar-Garza**, B. Hua, C.M. Williams, V. Nesterov, M.A. Omary

4:50 INOR **1242.** Role of specific and non-specific interactions in understanding the excited-state processes of transition-metal complex based photodrugs. **B. Dietzek**

5:10 INOR **1243.** Advanced ^{17}O MAS NMR methods to characterise the local environment in complex inorganic systems. D. Grekov, Y. Bouhoute, K.C. Szeto, N. Merle, I. Del Rosal, L. Maron, R. Gauvin, M. Taoufik, **L. Delevoye**

Section F

Moscone Center

2022

Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

B. Barry, A. Mukherjee, *Presiding*

1:30 INOR **1244.** Dual-modal MR/NIR fluorescent probes for zinc sensing applications. **E. Coakley**, N.J. Long

1:50 INOR **1245.** Coordination chemistry approach for lithium ion batteries. **W. Shi**, P. Cheng

2:10 INOR **1246.** Molecular engineering of ruthenium complexes for highly efficient dye-sensitized solar cells. **S. Aghazada**, M. Graetzel, M. Nazeeruddin

2:30 INOR **1247.** 1,2,3-Triazole-based chelating ligands under investigation: Tuning the donor strength. **L. Suntrup**, F. Stein, B. Sarkar

2:50 INOR **1248.** Development of molecular underground chemical tracers: Coordination chemistry of alkaline earth and transition metal salen-derivative precursors. **T.J. Boyle**, J.M. Sears, O. Staples, D. Perales, K. Wyss, J.A. Greathouse, R.A. Kemp

3:10 Intermission.

3:20 INOR **1249.** Understanding reactivities of transition metal compounds with ROS. **A. Mukherjee**

3:40 INOR **1250.** Mn(III) in an all O-donor ligand environment with fluorinated alkoxides. C. Kotyk, J. Henebry, C. Sun, J.L. Steele, Y. Chen, V.F. Oswald, J.W. Bacon, A.L. Rheingold, **L. Doerrer**

4:00 INOR **1251.** Synthesis and reactivity of redox-active molecular group 13 complexes. **T. Sherbow**, L.A. Berben

4:20 INOR **1252.** Dinuclear photoCORMS: Visible/near-infrared light activating CO release. **Z. Li**, A.E. Pierri, P. Huang, W. Gang, A. Iretskii, P.C. Ford

4:40 INOR **1253.** Design, synthesis and characterization of rhenium(I) tricarbonyl complexes derived from a-diimine coligand for bio-imaging applications. **J. Jimenez**, I. Chakraborty, P. Mascharak

5:00 INOR **1254.** Complexes with bisguanidine-type ligands towards oxidative additions across sp2-heteratom bonds. **B. Barry**, K. Feller, H. Schickel, J. Bruggen, J. Sanborn, R. Velcheck, J. Norman

Section G

Moscone Center

2024

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

T. T. Boron, P. Desrochers, *Presiding*

1:30 INOR **1255.** Coinage metal nanoclusters: Characterization and catalytic applications. **A.W. Cook**, T.W. Hayton

1:50 INOR **1256.** Temperature-Driven geometric conversion of solid-state polymorphs of a four-coordinate nickel(II) complex. **X.B. Powers**, K.B. Ghiassi, J.T. Greenfield, M.M. Olmstead, A.L. Balch

2:10 INOR **1257.** Side-on dioxygen complex of cobalt: Structure, reactivity, and conversion to bimetallic products. **D.E. DeRosha**, B.Q. Mercado, P.L. Holland, K.R. Rodgers

2:30 INOR **1258.** Synthesis and reactivity of imido and nitrido complexes of first row transition metals supported by tris(pyrazolyl)borate ligands. **D.C. Cummins**, K.H. Theopold, G.P. Yap

2:50 INOR **1259.** Synthesis and reactivity of new divalent bis(alkoxide) complexes. **T. Hollingsworth**, S. Groysman

3:10 Intermission.

3:20 INOR **1260.** Sweeter scorpionates incorporate carbohydrates into functional metal chelates. **P. Desrochers**, T. Clements

3:40 INOR **1261.** Cu(II) mixed-ligand polypyridyl complexes with 6-mercaptopurine: Synthesis, characterization and their cytotoxicity evaluations. **J.A. Obaleye**

4:00 INOR **1262.** Cytotoxicity studies of ruthenium(II) polypyridine compounds with a β-diketone ligand. J.A. Obaleye, **A.O. Rajee**, K.R. Dunbar

4:20 INOR **1263.** Withdrawn.

4:40 INOR **1264.** Anion effect on aluminum hydroxide cluster synthesis. **E. Eitrheim**, C.K. Perkins, B. Fulton, T. Forbes, D.A. Keszler

5:00 INOR **1265.** Controlling single-molecule magnetic behavior of two families of metallacrowns by modifying lanthanide choice or structural components. **T.T. Boron**, J.C. Lutter, C.I. Daly, C. Chow, A.H. Davis, A. Nimthong-Roldan, M. Zeller, J.W. Kampf, T. Mallah, C.M. Zaleski, V.L. Pecoraro

Section H

Moscone Center

3000

Environmental & Energy-Related Inorganic Chemistry

S. A. Koch, *Organizer*

M. Fieser, A. I. Nguyen, *Presiding*

1:30 INOR **1266.** Modeling the dissolution of transition metal oxide nanomaterials. **S.E. Mason**, **J. Bennett**

1:50 INOR **1267.** Understanding the mechanisms of CO_2 adsorption enhancement/degradation in all silica zeolites under wet conditions. **W. Jeong**, J. Kim

2:10 INOR **1268.** Photochemistry of a direct contact core-shell tandem photocatalyst for overall water splitting. **M.A. Melo**, F.E. Osterloh

2:30 INOR **1269.** Bioinspired electrocatalytic CO2 reduction using first-row transition metal catalysts. **E. Nichols**, C.J. Chang

2:50 INOR **1270.** Tunable, site-isolated Co_xO_4 oxygen-evolution catalysts in porous frameworks. **A.I. Nguyen**, K.M. Van Allsburg, M. Terban, M. Bajdich, J. Oktawiec, M.S. Ziegler, J.P. Dombrowski, K.V. Lakshmi, W. Drisdell, J. Yano, S. Billinge, T.D. Tilley

3:10 INOR **1271.** Aluminum doped $SrTiO_3$ nanocrystals as photocatalyst for overall water splitting under sunlight. **Z. Zhao**, F.E. Osterloh

3:30 Intermission.

3:40 INOR **1272.** Cationic dirhodium(II,II) complexes as dual action electrocatalysts for H^+ and CO_2 reduction. **S. Witt**, C. Turro

4:00 INOR **1273.** Progress towards catalytic ammonia splitting. **M.R. Smith**

4:20 INOR **1274.** Rational design of ruthenium(II) chromophores: Towards efficient photocatalytic proton reduction. **R.S. Khnayzer**, K. El Roz, F.N. Castellano

4:40 INOR **1275.** Catalytic decarbonylation of fatty acid esters. **M.E. Fieser**, A. John, L.A. Mitchell, B. Benson, L.T. Hogan, A.M. LaPointe, W.B. Tolman

5:00 INOR **1276.** Synthesis of Ni_2P nanoparticles supported r-GO composites for hydrodesulphurization applications. V. Tzitzios, M. Kartsiotis, V. Pillai, T. Anjana, G. Papavassiliou, T. Karagiannis, **S. Al Hassan**

5:20 INOR **1277.** Withdrawn.

Section I

Moscone Center

3010

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Catalysis: Characterization, Computations, & Reactivity

Cosponsored by PMSE

Financially supported by Dow-Dow Corning, ExxonMobil, STREM, Argonne National Lab, Northwestern University

A. Facchetti, T. Lohr, *Organizers*

M. Stalzer, *Presiding*

1:30 Introductory Remarks.

1:35 INOR **1278.** Oxidative water splitting with molecular, heterogenized and heterogeneous iridium catalysts. A. Bucci, I. Corbucci, L. Fagiolari, G. Menendez Rodriguez, G. Bellachioma, C. Zuccaccia, **A. Macchioni**

2:05 INOR **1279.** Cascade synthesis of nanoparticle-polymer composites. **M.A. Firestone**, B.S. Ringstrand, D.J. Williams, H.D. Magurudeniya, A. Joshi

2:35 INOR **1280.** DMF-stabilized single-nano-sized metal nanoclusters as catalyst for cross-coupling reactions. **Y. Obora**

3:05 Intermission.

3:15 INOR **1281.** Preparation of deuterated drugs through novel catalysis: Synthesis, purification, and preclinical data. **G.Y. Li**

3:45 INOR **1282.** Mechanistic insights into catalytic conversion methane and light alkanes over supported catalysts. **M. Neurock**

4:15 INOR **1283.** DFT approach for the investigation of single-site supported catalysts. **A. Motta**, M. Delferro, T. Lohr, T.J. Marks

Section J

Moscone Center

3012

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

T. J. Williams, *Presiding*

1:30 INOR **1284.** Highly electrophilic iridium species supported on a sulfated metal oxide for catalytic H/D incorporation. **R. Klet**, M. Delferro

1:50 INOR **1285.** Reactivity of *para*-benzoquinones with ^{iPr}PCPIrH$_4$: In search of new hydrogen acceptors. **M. Wilklow-Marnell**, W.W. Brennessel, W.D. Jones

2:10 INOR **1286.** Selective conversion of neat glycerol to lactic acid using a prolific catalyst. **I. Demianets**, Z. Lu, T.J. Williams

2:30 INOR **1287.** Platinum-catalyzed ligand-directed C-H functionalization reactions. **S. Huo**, D.C. McAteer, E. Javed

2:50 INOR **1288.** Synthesis of 2-alkynoates and 2-ynamides via palladium(II) catalysed oxidative carbonylation. **N.L. Hughes**, Q. Cao, C. Brown, M.J. Muldoon

3:10 INOR **1289.** Withdrawn.

3:30 INOR **1290.** Theoretical study of (hetero)aromatic fluorination catalyzed by palladium. **P. Fleurat-Lessard**, **M. Ponce Vargas**, J. Roger, C. Testa, J. Guilbaud, N. Pirio, J. Hierso

3:50 INOR **1291.** Room temperature conversion of CO_2 to methanol with nickel catalysis. Z. Lu, **T.J. Williams**

4:10 INOR **1292.** Relative thermodynamics of nickel hydride and formate complexes. **N.A. Eberhardt**, J.A. Krause, H. Guan

4:30 INOR **1293.** Computational study of dinuclear nickel catalyzed alkyne cyclotrimerization. **D. Kwon**, D. Ess

4:50 INOR **1294.** Synthesis of xanthene-bridged bis(iminopyridine) di-nickel complexes toward alkyne cyclotrimerization. **R. Hollingsworth**, R.L. Lord, S. Groysman

Section K

Moscone Center

3001

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

L. Geary, V. M. Iluc, *Presiding*

1:30 INOR **1295.** σ-Complexes of cobalt and copper. **Y. Lee**

1:50 INOR **1296.** Organometallic cationic dicopper complexes: Synthesis, mixed-valence, reactivity, and their role in catalysis. **M.S. Ziegler**, K.V. Lakshmi, T.D. Tilley

2:10 INOR **1297.** Using dispersion forces to isolate low-valent high-oxidation state copper complexes. **C. Wagner**, L. Tao, E.J. Thompson, T.A. Stich, J. Guo, J.C. Fettinger, L.A. Berben, R. Britt, S. Nagase, P.P. Power

2:30 INOR **1298.** C. C*-cyclometalated mesoionic NHC ligands in phosphorescent platinum(II) complexes. **J. Soellner**, T. Strassner

2:50 INOR **1299.** Adaptable chelating diphosphine ligand for the stabilization of elusive palladium and platinum alkylidenes. B. Barrett, **V.M. Iluc**

3:10 INOR **1300.** C. C* cyclometalated ruthenium NHC complexes. **D. Schleicher**, T. Strassner

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

3:30 INOR **1301.** Reactivity of nickel complexes bearing a $HN(CH_2CH_2P^iPr_2)_2$ ligand. **N.P. Nambukara Wellala**, J. Luebking, J.A. Krause, H. Guan

3:50 INOR **1302.** Enhanced photoluminescence quantum yields through excimer formation. **P. Piermaria**, T. Strassner

4:10 INOR **1303.** Synthesis of luminescent gold(III) cyclometalated complexes. **A.N. Sulicz**, A. Maity, T. Gray

4:30 INOR **1304.** Structural and electronic characterization of early stage Magnus-type organocobalt intermediates in the Pauson-Khand reaction via x-ray absorption spectroscopy. **L. Geary**

4:50 INOR **1305.** Delocalised chains and rings of ferrocenes. **L.E. Wilson**, T. Albrecht, N.J. Long

5:10 INOR **1306.** Selective C8-metalation of various purine nucleosides. **F. Kampert**, E.F. Hahn

5:30 INOR **1307.** Oxidation chemistry of palladium complexes with the smallest steric N-heterocyclic carbene, I Me (I Me = 1,3-Dimetylimidazole-2-ylidene). **E. Lee**

Section L

Moscone Center

3003

Main Group Chemistry

T. W. Hudnall, *Organizer*

T. Perera, *Presiding*

1:30 INOR **1308.** Antimony(III) secondary bonding interactions for anion binding. J. Qiu, **A.F. Cozzolino**

1:50 INOR **1309.** Novel reactivity of N-heterocyclic carbenes toward one-electron oxidants. **E. Lee**

2:10 INOR **1310.** Synthesis and photochemistry of N,N'- diamido-carbene – Supported Sb(V) and Bi(III) chloro complexes for solar fuel production. **T.A. Perera**, T.W. Hudnall

2:30 INOR **1311.** Stable N-heterocyclic carbene adducts of diphosphorus and carbon monoxide. **R.J. Gilliard**, R. Suter, Z. Benko, H. Grützmacher, J.D. Protasiewicz

2:50 INOR **1312.** Withdrawn.

3:10 INOR **1313.** Synthesis and characterization of stable emissive radicals and biradicals derived from singlet carbenes. R.N. Arias, C. Barragan, **T.W. Hudnall**

3:30 INOR **1314.** Withdrawn.

3:50 Intermission.

4:00 INOR **1315.** Hydrostannylation reactions of low valent tin(II) hydrides, $[ArSn(\mu\text{-}H)]_2$ (Ar = Ar^{Pri4} or Ar^{Pri6}, Ar^{Pri4} = C_6H_3-2,6-(C_6H_3-2,6-$^iPr_2$)$_2$ Ar^{Pri6} = C_6H_3-2,6-(C_6H_2-2,4,6-$^iPr_3$)$_2$) with acyclic and bicyclic olefins. **S. Wang**, M. McCrea-Hendrick, C.A. Caputo, C. Weinstein, J.C. Fettinger, P.P. Power

4:20 INOR **1316.** Sterically encumbering *N*-heterocyclic tetrylenes and their reactivity. **C. Weinstein**, Y. Zhu, G. Bertrand

4:40 INOR **1317.** Amido and alkyl complexes of magnesium, calcium and strontium containing highly fluorinated Tp' ligands. N. Romero, Q. Dufrois, **C. Dinoi**, M. Etienne

5:00 INOR **1318.** Synthesis of Lewis acid-stabilized calcium imides. **B.M. Wolf**, C. Maichle-Mössmer, R. Anwander

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Sponsored by PHYS, Cosponsored by INOR

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis

Devices, Assemblies & Hybrid Processes

Sponsored by CATL, Cosponsored by COLL, ENFL, I&EC and INOR

THURSDAY MORNING

Section A

Moscone Center

2009

Bioinorganic Chemistry

Proteins & Enzymes & Model Systems

S. A. Koch, *Organizer*

L. E. Cheruzel, S. A. Toledo, *Presiding*

8:00 INOR **1319.** Determination of differential orbital covalency of heme active sites by L-edge spectroscopy. **M.L. Baker**, B.K. Alpert, H. Cho, E. Denison, W.B. Doriese, J.W. Fowler, K.J. Gaffney, J. Gard, B. Gao, G.C. Hilton, K.D. Irwin, Y.I. Joe, C. Kenney, J. Knight, T. Kroll, S. Lee, D. Li, R. Marks, M. Minitti, K.M. Morgan, R.A. Mori, H. Ogasawara, G. O'Neil, D. Schmidt, D. Sokaras, D.S. Swetz, Y. Song, C.J. Titus, J. Ullom, T. Weng, C. Williams, J.J. Yan, B.A. Young, D. Nordlund, E.I. Solomon

8:20 INOR **1320.** Selective substrates C-H functionalization with light-driven P450 enzymes. **L.E. Cheruzel**

8:40 INOR **1321.** Unleashing a pendant base by reduction-induced hemilability in $[NiN_2S_2Fe(NO)_2]^{+/0}$ complexes. **P. Ghosh**, S. Ding, C. Hsieh, R.B. Chupik, N.S. Bhuvanesh, M.B. Hall, M.Y. Darensbourg

9:00 INOR **1322.** Model complexes of NiSOD and the factors that influence Ni redox cycling. **P.T. Truong**, T.C. Harrop

9:20 INOR **1323.** Cu(II) coordination differences in the amyloid-beta protein binding models GHK and DAHK result in varied conditional inter-peptidic metal exchange rate constants. **C.N. Beuning**, B. Mestre, C. Hureau, D.C. Crans

9:40 INOR **1324.** Hemilabile bridging thiolates as proton shuttles in bioinspired H_2 production electrocatalysts. **S. Ding**, P. Ghosh, A.M. Lunsford, N. Wang, N. Bhuvanesh, M.B. Hall, M.Y. Darensbourg

10:00 Intermission.

10:10 INOR **1325.** Interplay of copper and iron in NO release from Dinitrosyl Iron Complexes (DNICs). **R.B. Chupik**, D. Bruggeman, M. Maurice, J.A. Denny, M.Y. Darensbourg

10:30 INOR **1326.** Origins of the catalytic proficiency of cytochrome-based artificial metalloenzymes. **M. Garcia-Borras**, G. Jimenez-Oses, K.N. Houk

10:50 INOR **1327.** Expanding our understanding of Nickel-Acireductone Dioxygenase (Ni-ARD) through a family of structural analogues of the resting state of the enzyme. **S.A. Toledo**, D. Ivan, A. Sanchez, A.J. Gremillion, S. Sanchez, J.D. Green, V. Lynch

11:10 INOR **1328.** Withdrawn.

11:30 INOR **1329.** Structure-function relationships of Mn-containing super oxide dismutases (SOD) studied via quantum mechanical computational methods. **J.H. Rodriguez**

11:50 INOR **1330.** Merged heme and non-heme manganese co-factors for a dual anti-oxidant surveillance in photosynthetic organisms. **M. Bonchio**

Section B

Moscone Center

2011

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

L. Pan, L. Yang, *Presiding*

8:30 INOR **1331.** Structural flexibility, luminescence, and aurophilic interactions in crystals of the binuclear complexes $Au_2(Ph_2P(CH_2)_nPPh_2)_2X_2$ (n = 2-6, X = chloride and thiocyanate). **K.R. England**, K.B. Ghiassi, M.M. Olmstead, A.L. Balch

8:50 INOR **1332.** Water soluble cationic zinc lysine hydrochloride compound for spontaneous coating of znO on biomaterial surfaces. **L. Pan**

9:10 INOR **1333.** Luminescence and rearrangement of small poly-gold phosphine complexes. **D.T. Walters**, R. Babadi, X.B. Powers, K. Ghiassi, M.M. Olmstead, A.L. Balch

9:30 INOR **1334.** Designing and crystallographic characterization of trinuclear Cu(II) and dinuclear Zn(II) clusters. **M. Shahid**, F. Sama

9:50 INOR **1335.** First report of anagostic interaction in heteronuclear polyoxovanadate-Cu complex with highly selective sensing towards nitro explosives: X-ray, theoretical and TRF investigations. **M. Raizada**, **Z.A. Siddiqi**

10:10 Intermission.

10:20 INOR **1336.** Synthesis and characterization of copper complexes with Cu^ICu^I, $Cu^{1.5}Cu^{1.5}$ and $Cu^{II}Cu^{II}$ core structures supported by a flexible dipyridylamide ligand. **L. Yang**, E.P. McMoran

10:40 INOR **1337.** Binding modes and thermodynamics of iron and vanadium with amidoxime ligands. **B. Parker**, Z. Zhang, J. Arnold, L. Rao

11:00 INOR **1338.** Using the terminal metal-oxo bond as a reporter of electron donation from bicyclic guanidinate ligands to mid transition metals. **J. Olson**, D. Swenson, L. Messerle

11:20 INOR **1339.** Dual cavity tetracarboxamide host for anion and metal ion binding. **J. Lohrman**, H. Telikepalli, V.W. Day, K. Bowman-James

11:40 INOR **1340.** Light harvesting through photoswitchable molecules. **A. Rajput**, A.F. Cozzolino

‡ *Cooperative Cosponsorship*

Section C

Moscone Center
2016

Electrochemistry

B. L. Lucht, *Organizer, Presiding*

N. R. Neale, *Presiding*

8:00 INOR **1341.** Boron cluster-based ionic liquids for reversible electrodeposition. **R. Dziedzic**, S. Lee, J. Kleinsasser, B.D. Bosley, R.A. Kemp, T.L. Peng, V. Lavallo, **A.M. Spokoyny**

8:20 INOR **1342.** Effect of surface ligands on CoP for the hydrogen evolution reaction. **D. Ung**, B. Cossairt

8:40 INOR **1343.** Molecular surface modification of semiconductor photoelectrodes – A viable water splitting strategy? **N.R. Neale**, L.E. Garner, J. Gu, K.X. Steirer, J. Young, N.C. Anderson, E.M. Miller, J.A. Turner, A. Sellinger, T.G. Deutsch

9:00 INOR **1344.** High frequency resistivity: Determining fundamental photoelectrode properties in a complex world. **N.C. Anderson**, N.R. Neale

9:20 INOR **1345.** Redox-active deep eutectic solvents. **J.C. Goeltz**, L.N. Matsushima, D.G. Jones

9:40 INOR **1346.** Withdrawn.

10:00 INOR **1347.** Semiconductor-to-metal transition in rutile TiO_2 induced by tensile strain. **E. Benson**, E.M. Miller, S. Nanayakkara, B.A. Gregg

10:20 INOR **1348.** Deoptimizing the oxygen reduction reaction on doped amorphous TiO_2 coatings for corrosion inhibition. M. Groenenboom, R. Anderson, D. Horton, S. Policastro, **J.A. Keith**

10:40 INOR **1349.** Electrochemical detection of doxorubicin and salinomycin. **J.A. Nikles**, B.J. McCormick, S. Pan, D.E. Nikles

11:00 INOR **1350.** Fluorescence spectroelectrochemistry of integrated anthraquinone-polyether macrocycles. **A.G. Sykes**

11:20 INOR **1351.** Electroreduction pattern of quinone units in pillar[5-n]arene[n] quinones. **M. Rashvand Avei**, A.E. Kaifer

11:40 INOR **1352.** Electro-thermochemical cycling process for high-yield ammonia synthesis from N_2 and H_2O at atmospheric pressure. **J.M. McEnaney**, A.R. Singh, J.A. Schwalbe, J. Kibsgaard, J.C. Lin, M. Cargnello, T.F. Jaramillo, J.K. Norskov

Section D

Moscone Center
2018

Solid-State Inorganic Chemistry

C. G. Lugmair, V. Poltavets, *Organizers*

J. Brgoch, K. Kovnir, *Presiding*

8:30 INOR **1353.** Decoupled electronic and phonon transport in complex chalcogenides: A substructure approach. **K. Biswas**

8:45 INOR **1354.** Thermoelectric performance of Zintl phase $Yb_{2-x}Eu_xCdSb_2$ exhibiting low thermal conductivity. **J. Cooley**, P. Promkhan, S. Gangopadhyay, D. Donadio, S. Kauzlarich

9:00 INOR **1355.** Stabilization of extraordinary off-stoichiometric Bi_2Te_3 for enhancing n-type thermoelectric performance. **I. Chung**

9:15 INOR **1356.** Synthesis, structure, and properties of new Si-As framework compounds. **K. Woo**, J. Dolyniuk, K. Kovnir

9:30 INOR **1357.** High-throughput experimental approach to find new transition metal ternary chalcogenides. **A. Bhutani**, A. Narayan, J.N. Eckstein, L.K. Wagner, D. Shoemaker

9:45 INOR **1358.** Crystal chemistry and magnetism of complex compounds with Zn-P frameworks. **K. Kovnir**

10:00 INOR **1359.** $Mg_{0.5}B_5C$ carbaboride as Mg-ion intercalation cathode with redox active anions by first-principles calculations. **V. Poltavets**, J.D. Davis, M. Johannes

10:15 INOR **1360.** Elucidating the mechanism of high-rate and high-capacity lithium-ion intercalation in bulk complex transition metal oxides. **K.J. Griffith**, A. Forse, J.M. Griffin, C.P. Grey

10:30 Intermission.

10:45 INOR **1361.** Withdrawn.

11:00 INOR **1362.** Design and synthesis of novel rare earth kagome materials: Applications in geometric magnetic frustration. **M.B. Sanders**, R.J. Cava

11:15 INOR **1363.** Development of a low-temperature solvothermal route to a variety of novel iron chalcogenides. **J.T. Greenfield**, K. Kovnir

11:30 INOR **1364.** Synthesis and low-temperature properties characterization of superconducting $Ni_{1-x}Bi$. **K.M. Powderly**, S.M. Clarke, A.J. Rettie, C. Malliakas, D.E. Freedman

11:45 INOR **1365.** Rapid microwave preparation of new earth abundant magnetocaloric materials. **J. Grebenkemper**, J.D. Bocarsly, E. Levin, R. Seshadri

12:00 INOR **1366.** *In situ* and real-time monitoring of mechanochemical ZIF8 synthesis via gas pressure measurements. **I. Brekalo**, C. Mottillo, K.T. Holman, T. Friscic

12:15 INOR **1367.** Mechanistic insights into the chemical and electronic properties of dielectric materials exposed to chemical warfare agents and their structural analogs. **J.R. Soliz**, A.L. Tang, W.O. Gordon, A. Balboa, A.J. Hauser, S.R. Padovani

Section E

Moscone Center
2020

Inorganic Catalysts

S. A. Koch, *Organizer*

M. T. Kieber-Emmons, X. Zhao, *Presiding*

8:30 INOR **1368.** Reactivity of the $Mo_2O_2S_4(DMF)_3$ complex with cyanide and catalytic conversion of cyanide to thiocyanate. **S.G. Suman**, J. Gretarsdottir, R. Bjornsson

8:50 INOR **1369.** Electro- and photolytic hydrogen production catalyzed by molecular Co complexes with pentadentate ligands in aqueous solution. **X. Zhao**, P. Wang, Y. Sun, L. Duan, M. Long, D. Reese, A. Bah, C. James, G. Liang, C.E. Webster

9:10 INOR **1370.** Alcoxysilanes production from silica and dimethylcarbonate promoted by alkali bases: A DFT investigation of the reaction mechanism. **V. Butera**, Y. Choe, N. Fukaya, J. Choi, K. Sato

9:30 INOR **1371.** Dehydrogenation of ammonia borane through the third equivalent. X. Zhang, **L. Kam**, T.J. Williams

9:50 INOR **1372.** Synthetic approaches for cyclic biodegradable polyesters using ligated tin(II) complexes. **K. Phomphrai**, P. Piromjitpong, P. Wongmahasirikun

10:10 Intermission.

10:20 INOR **1373.** Synthesis and characterization of cyclic polyester: Effect of alkoxy side chains on Shiff's base ligand of tin(II) complexes. **P. Wongmahasirikun**, K. Phomphrai

10:40 INOR **1374.** Rh and Pt nanoparticles stabilized by phosphine functionalized silica for selective hydrogenation reactions. **C. Claver**, J. Llop, C. Godard, M. Taoufik

11:00 INOR **1375.** Efficient and selective oxidation of sulfur mustard using singlet oxygen generated by a pyrene-based metal–organic framework. **Y. Liu**, C.T. Buru, A. Howarth, J. Mahle, J. Buchanan, J.B. DeCoste, J.T. Hupp, O.K. Farha

11:20 INOR **1376.** Electrocatalytic water oxidation by a dicopper dihydroxide precatalyst reveals dinuclear intermediates. **M.T. Kieber-Emmons**, S.J. Koepke, P.E. VanNatta, A. Shrestha

11:40 INOR **1377.** Highly controllable syngas (H_2 + CO) production through immobilized dual molecular Re(I)/Co(III) catalyst on a ternary TiO_2 hybrid system. J. Lee, D. Won, W. Jung, **H. Son**, C. Pac, S.O. Kang

Section F

Moscone Center
2022

Lanthanide & Actinide Chemistry

Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

J. F. Corbey, S. Demir, L. S. Natrajan, *Presiding*

8:30 INOR **1378.** Solution synthesis and CO_2 reactivity of a rare Sc^{2+} complex, $[Sc(NR_2)_3]^{1-}$ (R = $SiMe_3$). **D. Woen**, G. Chen, J.W. Ziller, T.J. Boyle, F.U. Furche, W.J. Evans

8:50 INOR **1379.** Synthesis, structure, and reactivity of complexes containing +2 ions of late lanthanide metals in tris(silylamide) coordination environments, $\{Ln[N(SiMe_3)_2]_3\}^{1-}$. **A. Ryan**, J.W. Ziller, W.J. Evans

9:10 INOR **1380.** Metalation of C–H bonds by $Cp^*_2Y(\mu\text{-}Me)_2MMe_2$ (M = Al, Ga). **M. Bonath**, C. Maichle-Mössmer, R. Anwander

9:30 INOR **1381.** Radical-Bridged lanthanide single-molecule magnets with high blocking temperatures. **S. Demir**, J.R. Long

9:50 Intermission.

10:00 INOR **1382.** Synthesis and reactivity of organometallic divalent lanthanide compounds using a tris(aryloxide) mesitylene ligand. **C. Palumbo**, D.P. Halter, M.E. Fieser, H.S. La Pierre, J.W. Ziller, M. Gembicky, K. Meyer, W.J. Evans

10:20 INOR **1383.** Binding preferences of uranyl with cyclic imide dioximes: A theoretical investigation. **D.A. Penchoff**, C. Peterson, G.K. Schweitzer, D.M. Jenkins, R.J. Harrison

10:40 INOR **1384.** Structural exploration of trivalent f element-containing species of interest for liquid-liquid extraction processes. **J.F. Corbey**, B.K. McNamara, B.M. Rapko, J.M. Schwantes

11:00 Intermission.

11:10 INOR **1385.** Optical spectroscopic foray into the redox chemistry of the early actinides. M. Andrews, S. Woodall, A. Swinburne, J. Lloyd, A. Ward, S. Botchway, **L.S. Natrajan**

11:30 INOR **1386.** Synthesis and magnetic characterization of trinuclear, radical-bridged lanthanide single-molecule magnets. **C.A. Gould**

11:50 INOR **1387.** Hydropyridinonate ligands: From iron(III) to berkelium(IV) chemistry. **G. Deblonde**, D. An, P.B. Rupert, R.K. Strong, R.J. Abergel

Section G

Moscone Center
2024

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

H. Guan, S. M. Kilyanek, *Presiding*

8:30 INOR **1388.** Palladium POCOP-pincer complexes: Catalysis in reduction of CO2 with boranes. A. Adhikary, J.A. Krause, **H. Guan**

8:50 INOR **1389.** Using stopped-flow kinetics as a mechanistic probe for the insertion of carbon dioxide into metal-hydride bonds. **J. Heimann**, N. Hazari

9:10 INOR **1390.** Role of LiCl in generating soluble organozinc reagents. C. Feng, D. Cunningham, **Q. Easter**, S. Blum

9:30 INOR **1391.** Filling the gap: Exploration of organoactinide catalysts with amine boranes reveal highly active catalysts and unique structural motifs. **K. Erickson**, B. Scott, P. Dub, J.L. Kiplinger

9:50 INOR **1392.** Catalysis, carbon-hydrogen, and carbon-carbon bond activation with PNP Pincer-supported group 3 and lanthanide alkyl complexes. **D.S. Levine**, T.D. Tilley, R.A. Andersen

10:10 INOR **1393.** Unexpected proton transfer mechanism in the racemization of lactic acid catalyzed by lactate racemase: A DFT study. B. Qiu, **X. Yang**

10:30 INOR **1394.** Mechanism based oligomerization catalysis for upgrading a-olefins to produce specialty fuels and chemicals. **T.N. Gunasekara**, M.M. Abu-Omar

10:50 INOR **1395.** Mechanistic studies of the deoxydehydration of polyols by group VI transition metal catalysts. **S.M. Kilyanek**, R. Tran, K.A. DeNike

11:10 INOR **1396.** Isolation of key intermediates in Mo-catalyzed hydrosilylation. **K. Mandla**, J.S. Figueroa

11:30 INOR **1397.** Proton and electron transfer by redox-active aluminum complexes for small molecule reduction. **E.J. Thompson**, T. Sherbow, L.A. Berben

11:50 INOR **1398.** Norbornenyl-Acyl-Rhodium(III) complex as a likely intermediate in the catalytic hydroacylation of norbornadiene. **M.A. Huertos**

Section H

Moscone Center
3000

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

P. Deria, M. C. So, *Presiding*

8:30 INOR **1399.** Novel magnetic composite materials: Metal-organic frameworks as hosts for molecular nanomagnets. **D. Aulakh**, J. Pyser, X. Zhang, A. Yakovenko, K.R. Dunbar, M. Wriedt

8:50 INOR **1400.** Molecular mechanisms of spin crossover in the {Fe(pz)[Pt(CN)4]} MOF upon guest adsorption. **H. Pham**, F. Paesani

9:10 INOR **1401.** Multifunctional MOFs materials platform for biomedical applications. **D.F. Sava Gallis**, L.E. Rohwer, M.A. Rodriguez

9:30 INOR **1402.** Control over electronic delocalization and conductivity in mixed-valence semiquinoid frameworks. **M.E. Ziebel**, L.E. Darago, J.R. Long

9:50 INOR **1403.** Topology-Dependent photophysical properties of zirconium-based metal-organic frameworks. **P. Deria**

10:10 INOR **1404.** Withdrawn.

10:30 Intermission.

10:45 INOR **1405.** Interrogation of charge transport by gas sorption in metal-organic frameworks. **M. Aubrey**, M. Kapelewski, J. Melville, J.R. Long

11:05 INOR **1406.** Isolation of metalloporphyrin dioxygen adducts in metal-organic frameworks. **A. Gallagher**, D. Harris, J. Anderson, M. Kelty

11:25 INOR **1407.** Ultra-sensitive detection of mycotoxins by a luminescent metal-organic framework. **Z. Hu**, W.P. Lustig, J. Zhang, C. Zheng, H. Wang, S.J. Teat, Q. Gong, N. Rudd, J. Li

11:45 INOR **1408.** Uptake mechanism, diffusion, and binding energetics of chemical warfare agent simulants within MOFs. **C.H. Sharp**, J. Abelard, A. Plonka, Q. Wang, A. Frenkel, W. Guo, C.L. Hill, D. Troya, J.R. Morris

12:05 INOR **1409.** Preliminary electrochemical studies on effects of linker length and metal nodes on redox hopping in layer-by-layer assembled metalloporphyrin metal-organic framework-like thin films. **M.C. So**, K. Hara, J.T. Hupp, O.K. Farha

Section I

Moscone Center
3010

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

S. Fischer, J. A. Mason, *Presiding*

8:00 INOR **1410.** Design and synthesis of $WO(OR)_3L$ complexes as precursors for chemical vapor deposition of WO_x thin films. **X. Su**, D.C. Bock, T.J. Anderson, L. McElwee-White

8:20 INOR **1411.** Quantitative control of metal doping in TiO_2 nanocrystals. **S. Mia**, S. Varapragasam, C. Balasanthiran, J.D. Hoefelmeyer

8:40 INOR **1412.** Exploring metal oxide nanostructure synthesis mechanisms using *In situ* TEM. **L. Yu**, R. Han, H. Djieutedjeu, A. Patel, B.S. Guiton

9:00 INOR **1413.** Insights into solution-processed metal oxide thin film formation mechanisms through investigations of non-thermal energy sources for annealing. **E. Cochran**, D. Park, M. Kast, P. Plassmeyer, C. Page, D.W. Johnson, D.A. Keszler, S.W. Boettcher

9:20 INOR **1414.** Structure of sub-nm oxides synthesized by atomic layer deposition: From isolated cations to bulk-like structure. **A. Yanguas-Gil**, T. Wu, J. Elam

9:40 Intermission.

9:55 INOR **1415.** Precise control over the morphology and dopant distribution in colloidal metal oxide nanocrystals. **A. Singh**, D.J. Milliron

10:15 INOR **1416.** Nanoparticle treated filters for sequestration of radioactive analytes. **S. Hunyadi Murph**

10:35 INOR **1417.** DNA-mediated assembly of stimuli-responsive colloidal crystals. **J.A. Mason**, C. Laramy, C. Lai, M. Obrien, Q. Lin, V.P. Dravid, G.C. Schatz, C.A. Mirkin

10:55 INOR **1418.** Exploring the morphology transition from Li/Na $\{U_{24}Pp_{12}\}$ to Na/K $\{U_{24}Pp_{12}\}$ uranyl peroxide nanocluster. **Y. Gao**, M. Dembowski, J. Szymanowski, W. Yin, S. Chuang, P.C. Burns, T. Liu

11:15 INOR **1419.** Shape control of multi-layer lanthanide-doped NaYF4 nanocrystals by exploiting the shell growth dynamics. **S. Fischer**, A. Alivisatos

11:35 INOR **1420.** Control and quantification of local polarity in nano-confined systems. **D. Singappuli-Arachchige**, J. Manzano, L.M. Sherman, I.I. Slowing

11:55 INOR **1421.** Morphology, electropinnability, and crystalline phase study of SiO_2/TiO_2 composite ceramic nanofibers using sol-gel chemistry. **F. Huang**, B. Motealleh, C.J. Cornelius

Section J

Moscone Center
3012

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

E. G. Gillan, M. B. Ross, *Presiding*

8:30 INOR **1422.** Translation of ligand-centered hydrogen evolution reaction activity and mechanism from homogeneous to solid surfaces. **W. Zhang**, R.M. Buchanan, C.A. Grapperhaus

8:50 INOR **1423.** Monitoring surface species during carbon dioxide reduction using in situ Raman spectroscopy. **M.B. Ross**, Y. Li, C. Dinh, E. Sargent, P. Yang

9:10 INOR **1424.** Withdrawn.

9:30 INOR **1425.** Synthesis and catalytic reactions with 3d and 4d phosphorus-rich metal phosphides. **E.G. Gillan**

9:50 INOR **1426.** Comparison and structural modulation of cobalt amino porphyrin complexes for electrochemical reduction of CO_2. **M. Abdinejad**, H. Kraatz, X. Zhang

10:10 Intermission.

10:25 INOR **1427.** Comparative electrocatalytic activities of bimetallic oxides and carbides of iron, nickel and cobalt with tungsten and molybdenum as the second transition metal. **Y.N. Regmi**, B.M. Leonard

10:45 INOR **1428.** Molecular Ni-complex containing tetrahedral nickel selenide core as highly efficient electrocatalyst for oxygen evolution reaction in alkaline medium. **M. Nath**, J. Masud, P. Kyritsis

11:05 INOR **1429.** Chemistry of chromium carbide mono and bimetallic systems: Synthesis and electrocatalytic activity. **B.M. Leonard**, C. Wan, S. Schmuecker

11:25 INOR **1430.** Novel catalytic materials for energy and environment investigating transition metal chalcogenides for efficient oxygen evolution electrocatalysis: The effect of covalency and lattice directionality. **M. Nath**

Section K

Moscone Center
3001

Coordination Chemistry: Characterization & Applications

S. A. Koch, *Organizer*

K. V. Waynant, *Presiding*

8:30 INOR **1431.** Water-soluble thiophene-based fluorescent mercury-sensors. **A.K. Shigemoto**, C. Virca, A. Thompson, J. Dayton, T. McCormick

8:50 INOR **1432.** Coordination chemistry approaches for rational vanadium(IV) qubit design. **C. Yu**, M. Graham, J. Zadrozny, D.E. Freedman

9:10 INOR **1433.** ^{1}H Relaxometric approach to determining the thermodynamic and kinetic stabilities of Mn(II) complexes. **D.W. Laorenza**, T.D. Westmoreland

9:30 INOR **1434.** $[MoO(S_2)_2L]^{1-}$ (L = picolinate or pyrimidine-2-carboxylate) Complexes as MoS_x inspired electrocatalysts for hydrogen production in aqueous solution. **B. Garrett**, C.M. Hadad, Y. Wu

9:50 Intermission.

10:00 INOR **1435.** Synthesis, properties, and reactivity of d^3 terminal–oxo molybdenum and tungsten complexes. **H.B. Vibbert**, M.D. Hopkins

10:20 INOR **1436.** Anion-Incarcerating nanojars: Solution and solid-state characterization and selective extraction of anions from water. **G. Mezei**, B. Ahmed

10:40 INOR **1437.** Pentadentate and hexadentate pyridinophane ligands support reversible Cu(I)/Cu(II) redox couples. **A. Wessel**, L.M. Mirica

11:00 INOR **1438.** Mono vs dual metal catalysis. **A. Poater**

11:20 INOR **1439.** Rational catalyst design of first-row d^8 complexes for the electrocatalytic reduction of CO_2. **A. Osterich**er, M. Reineke, C.P. Kubiak

11:40 INOR **1440.** Tripodal pyrazole ligands and analogs for selective ammonium and actinide extraction and sensing. **T.M. Jonah**, L. Mathivathanan, S. Kandel, R.G. Raptis, K. Kavallieratos

12:00 INOR **1441.** Coordination studies of arylazothioformamide ligands with transition metals in varying oxidation states for removal of trace metal impurities. **K.V. Waynant**, N.A. Johnson, S.R. Wolfe, J.G. Moberly, M.F. Roll

Section L

Moscone Center
3003

Organometallic Chemistry: Applications to Materials & Polymer Science

N. S. Radu, *Organizer*

C. E. Knapp, *Presiding*

8:30 INOR **1442.** Preparation of multiblock copolymers via stepwise addition polymerization of L-lactide and trimethylene carbonate. **M. Abubekerov**, J. Wei, P. Diaconescu

8:50 INOR **1443.** Copper ligand and anion effects on the kinetics of photo-induced copper(I) catalyzed azide-alkyne cycloaddition polymerizations. **B. El-Zaatari**, S. Cole, C.J. Kloxin

9:10 INOR **1444.** Application of amino and imino pyridine iron(II) catalysts in atom transfer radical polymerization. **S.E. Jenny**, L.M. Thierer, M.R. Donley, L.M. Round, N.A. Piro, W.S. Kassel, D.L. Zubris

9:30 INOR **1445.** Optimization of iron-loaded nanoparticles for T_1-weighted MRI contrast enhancement. **T.B. Ditri**, Y. Li, Z. Wang, Y. Huang, Y. Xie, M. Botta, J.D. Rinehart, N.C. Gianneschi

9:50 INOR **1446.** Porous flexible $Cu_2(pzdc)_2(L)$ [pzdc = 2,3-pyrazinedicarboxylate; L = 1,3-bis(imidazol-1-yl) benzene or 1,3-bis(4-pyridyl)propane] pillared-layer structures. **R.R. Arrieta-Perez**, J.N. Primera-Pedrozo, M.E. Marcano-Gonzalez, J. Exley, J.A. Hogan, D.L. Jan, A.J. Hernandez

10:10 INOR **1447.** Nitrogen-doped Polycyclic Aromatic Hydrocarbons (PAHs) *via* titanocene-mediated dinitrile coupling. **G.R. Kiel**, T.D. Tilley

10:30 Intermission.

10:35 INOR **1448.** Block copolymers synthesized by redox-switchable catalysis. **S. Quan**, P. Diaconescu

10:55 INOR **1449.** Co-supported tandem catalysts for production of linear low density polyethylene. **D. Aluthge**, A. Sattler, J.E. Bercaw, J.A. Labinger

11:15 INOR **1450.** Designer copper precursors and their use in functional materials. **C.E. Knapp**, S.P. Douglas, E.A. Metcalf

11:35 INOR **1451.** Cationic iridium(III) complexes bearing 2-aryl substituted oxazolo[4,5-f][1,10]phenanthroline (N. N) ligands: Synthesis, crystal structure, photophysics and application for reverse saturable absorption. **X. Zhu**, W. Sun

11:55 INOR **1452.** Reversible electropolymerization of nickel azobispyridine complexes based on redox mediated ligand exchange. **N. Clayman**, A. Rudenko, R.M. Waymouth

‡ *Cooperative Cosponsorship*

THURSDAY AFTERNOON

Section A

Moscone Center
2009

Coordination Chemistry: Synthesis & Characterization

S. A. Koch, *Organizer*

L. Cronin, J. M. Sears, *Presiding*

1:30 INOR **1453.** Solving topological puzzles in tetramethylcyclam-supported oxoiron(IV) chemistry. **J. Prakash**, G. Rohde, L. Que

1:50 INOR **1454.** Synthesis, electronic structure and reactivity of square-planar open shell iridium imido complexes. **M. Kinauer**, S. Schneider

2:10 INOR **1455.** Assembling complex inorganic clusters using a programmable networked one-pot reaction array. **L. Cronin**

2:30 INOR **1456.** Synthesis and reactivity of six-membered N-heterocyclic thiones and selones. **J.J. Flanagan**, D. Rabinovich

2:50 INOR **1457.** Exploration of $M[SNS]_2$ (M = Mo, W) as redox-active metalloligands in heteromultimetallic systems. **M. Wojnar**, A.F. Heyduk

3:10 Intermission.

3:20 INOR **1458.** Ligand-based redox chemistry in transition metal complexes of linear oligopyrroles. **R. Gautam**, E. Tomat

3:40 INOR **1459.** Scandium salt dehydration for recycling efforts. **J.M. Sears**, T.J. Boyle, F.A. Fasulo

4:00 INOR **1460.** Single-molecule magnetism in a series of two-coordinate ML_2 transition metal complexes. **P. Bunting**, J.R. Long

4:20 INOR **1461.** Electronic conductivity and magnetic ordering in mixed-valence $M(1,2,3\text{-triazolate})_2$ (M = $Cr^{II/III}$, $Fe^{II/III}$) metal-organic frameworks. **J.G. Park**

4:40 INOR **1462.** Deconvoluting the relative oxidation states in hexanuclear cobalt clusters. **R. Hernandez Sanchez**, A. Champsaur, D. Paley, B. Choi, M.L. Steigerwald, C.P. Nuckolls

Section B

Moscone Center
2011

Inorganic Catalysts

S. A. Koch, *Organizer*

C. J. Stromberg, *Presiding*

1:30 INOR **1463.** Hierarchical structured TiO_2 nanofibrous membranes with enhanced flexibility and photocatalytic activity. **M. Zhang**, J. Song, B. Ding

1:50 INOR **1464.** Computational investigations of ruthenium with promoters for Fischer-Tropsch processes. **E.N. Brothers**, S. Moncho, B.G. Janesko

2:10 INOR **1465.** Steric, electronic, and geometric effects on the ring opening transesterification polymerization mechanism for sustainable poly(lactones) with aluminum and zinc alkoxide catalysts. **D.E. Stasiw**, A.M. Luke, T. Rosen, M. Mandal, C.J. Cramer, M. Kol, W.B. Tolman

2:30 INOR **1466.** First principles study of sulfinamido-olefin ligands in the rhodium-catalyzed addition of arylboronic acids to ketones. **P. Miro**, R. Recio, I. Fernandez

2:50 INOR **1467.** Electrochemical reduction of CO_2 catalyzed by Re(pyridine-oxazoline)$(CO)_3Cl$ complexes. **J. Nganga**

3:10 Intermission.

3:20 INOR **1468.** One-pot synthesis of Pt nanoparticles supported by graphene nanoribbons with enhanced catalytic performance towards 4-nitrophenol reduction. **D.A. Martinez**, S. Wang, W. Chiang

3:40 INOR **1469.** Important role of the electrode surface in the electrochemical reduction of CO_2 by Ni-cyclam. **A. Zhanaidarova**

4:00 INOR **1470.** Copper tungstate microcrystals as photocatalyst for water oxidation under visible light. **Z. Wu**, F.E. Osterloh

4:20 INOR **1471.** Ultrafast dynamics of cyano functionalized [FeFe]-hydrogenase model compounds. **C.J. Stromberg**, E.J. Heilweil

4:40 INOR **1472.** Selective H_2 or formate production from CO_2 and water: Mechanistic insights achieved from ligand design. **N.D. Loewen**, L.A. Berben

Section C

Moscone Center
2016

Lanthanide & Actinide Chemistry

Cosponsored by WCC

A. De Bettencourt Dias, *Organizer*

E. Borbas, J. H. Farnaby, A. F. Martins, *Presiding*

1:30 INOR **1473.** Highly axial magnetic anisotropy in a N_3O_5 dysprosium(III) coordination environment generated by a merocyanine ligand. P. Selvanathan, B. Le Guennic, S. Rigaut, K. Bernot, **L. Norel**

1:50 INOR **1474.** Series of Dy^{3+} single-molecule magnets with terminal alkoxide ligands that promote large barriers to magnetic relaxation. **L.E. Darago**, J.R. Long

2:10 INOR **1475.** F-element complexes with phosphinimide ligands: Probing metal-ligand covalency using ^{31}P NMR Spectroscopy. **S. Younger-Mertz**

2:30 INOR **1476.** Excitation- and emission-based multiplexing with near infrared-emitting luminescent lanthanide complexes using red-light excitation. R. Xiong, **E. Borbas**

2:50 Intermission.

3:00 INOR **1477.** Investigating the subtle variations in uranyl and neptunyl oxo reactivity through the characterization of crown ether complexes. **M.C. Basile**, E.R. Cole, T. Forbes

3:20 INOR **1478.** Using bandgap tuneable capped nanoparticles to sensitize emissive Ln^{III} ions. **R.A. Tigaa**, G.J. Lucas, S. Silva-Hernandez, J.H. Monteiro, A. De Bettencourt Dias

3:40 INOR **1479.** Imaging L-lactate by CEST using paramagnetic shift reagents. **A.F. Martins**, L. Zhang, **A. Sherry**

4:00 Intermission.

4:10 INOR **1480.** Synthesis of multi-metallic lanthanide and actinide complexes from organometallic building-blocks. **J.H. Farnaby**

4:30 INOR **1481.** Spectroscopic and computational characterization of Eu(III)-oxalate precipitation processes. **W.C. Isley**, S. Kathmann, Z. Wang, G.B. Hall, S. Chatterjee, E.J. Bylaska, T. Meadows, G.J. Lumetta

4:50 INOR **1482.** Synthesis and redox behavior of uranium amidinate complexes. **M. Straub**, S. Hohloch, S.G. Minasian, J. Arnold

Section D

Moscone Center
2018

Main Group Chemistry

T. W. Hudnall, *Organizer*

J. D. Hoefelmeyer, T. Hudnall, *Presiding*

1:30 INOR **1483.** Lewis acidic antimony: Application as a non-innocent ligand for the activation of platinum catalyst. **D. You**, H. Yang, F. Gabbaï

1:50 INOR **1484.** Fluorescent frustrated Lewis pairs for the coordination and functionalization of small molecules. **Z.M. Heiden**, I.A. Kieffer, R.J. Allen

2:10 INOR **1485.** Ambiphilic molecules with (quinolin-8-yl) groups on electrophiles. J. Son, S.R. Tamang, J.I. Fostvedt, **J.D. Hoefelmeyer**

2:30 INOR **1486.** Reactivity of Verkade's superbase with various strong lewis acids. **S. Mummadi**, D. Unruh, C. Krempner

2:50 INOR **1487.** Synthesis and application of novel polyhalides. **B. Schmidt**, K. Sonnenberg, F. Redeker, R. Brückner, S. Riedel

3:10 INOR **1488.** Solvent-free mechanochemical s-block chemistry: When synthesis and reactivity don't follow the rules. N.R. Rightmire, N.C. Boyde, **T.P. Hanusa**

3:30 Intermission.

3:40 INOR **1489.** Withdrawn.

4:00 INOR **1490.** Ultrashort beryllium-beryllium distances in molecular clusters. **X. Wang**

4:20 INOR **1491.** Boron-based donor-spiro-acceptor compounds as TADF emitters. **A. Lorbach**

4:40 INOR **1492.** Synthesis and characterization of polyborafluorenes, a novel boron doped varient of polyparaphenylene. **I.A. Brettell-Adams**, P. Rupar

5:00 INOR **1493.** Novel antimony-containing heterocycles synthesized via a Zr-transfer strategy. **A.M. Christianson**, F.P. Gabbai, E. Rivard

5:20 INOR **1494.** Cationic N-phosphoranimine ionic liquids. **J.R. Klaehn**, J.S. McNally, N. Arulsamy, H.W. Rollins, E.J. Dufek

5:40 INOR **1495.** Solid, stable, soluble, and stoichiometric oxidizing agents: Hydrogen peroxide and di(hydroperoxy)alkane adducts of phosphine oxides. **J. Bluemel**

Section E

Moscone Center
2020

Organometallic Chemistry: Catalysis

N. S. Radu, *Organizer*

J. M. Camara, *Presiding*

1:30 INOR **1496.** Cationic palladium(II) complexes for the catalytic Wacker-typeo oxidation of styrenes to ketones using O_2 as the terminal oxidant. H. Chai, Q. Cao, L.M. Dornan, **M.J. Muldoon**

1:50 INOR **1497.** Imparting nobility to first-row metal-hydrides: Unusual anionic Ni-H stabilized by Lewis acidic metal supports and their role in catalytic carbon dioxide hydrogenation. **R. Cammarota**, C. Lu

2:10 INOR **1498.** Withdrawn.

2:30 INOR **1499.** Metallocenes adsorbed on silica and activated carbon: Solid-State NMR and catalysis. **J. Bluemel**, K.J. Cluff

2:50 INOR **1500.** Synthesis of aziridines at low alkene loadings catalyzed by a chromium(III) tetracarbene complex. **C. Keller**, A. Cramer, G. Elpitiya, J. Kern, S. Roy, D.M. Jenkins

3:10 INOR **1501.** Withdrawn.

3:30 INOR **1502.** Mechanistic study of cyclotrimerization of alkynes via a two-coordinate iron complex. **R. Witzke**, T.D. Tilley

3:50 INOR **1503.** Mechanism of Wacker-type oxidation of terminal olefins with cationic Pd(II) complexes using hydrogen peroxide. **L.M. Dornan**, K.L. Walker, R.M. Waymouth, M.J. Muldoon

Section F

Moscone Center
2022

Chemistry of Materials: Metal Organic Frameworks

C. G. Lugmair, *Organizer*

C. McGuirk, *Presiding*

1:30 INOR **1504.** Polymer/Metal-organic-framework composite nanoparticle for gas separation: Rational design and theoretical analysis of core-shell structure. **K. Xie**, Q. Fu, P. Webley, G.G. Qiao

1:50 INOR **1505.** Methane adsorption in a flexible iron metal-organic framework with intrinsic heat management. **J. Oktawiec**, J.A. Mason, M.K. Taylor, M.R. Hudson, J. Rodriguez, J. Bachman, M.I. Gonzalez, A. Cervellino, A. Guagliardi, C.M. Brown, P. Llewellyn, N. Masciocchi, J.R. Long

2:10 INOR **1506.** Cooperative and reversible chemisorptive capture of carbon disulfide in diamine-appended metal-organic frameworks. **C. McGuirk**, R.L. Siegelman, P.J. Milner, J.R. Long

2:30 INOR **1507.** Computing adsorption properties of structurally deformed metal organic frameworks using a feature space map. **W. Jeong**, D. Lim, S. Kim, A. Harale, M. Yoon, M.P. Suh, J. Kim

2:50 INOR **1508.** Enhancing the uptake of oxygen in metal-organic frameworks. **J.B. DeCoste**, T.M. Tovar, I.O. Iordanov, A.M. Ploskonka, G.W. Peterson

3:10 INOR **1509.** Thermodynamically directed method to tether alkylamine into metal-organic frameworks for CO_2 capture. **H. Li**, H. Zhou

3:30 Intermission.

3:45 INOR **1510.** Record selectivity for olefin/paraffin separations in a metal-organic framework. **M. Kapelewski**, J. Bachman, J.R. Long

4:05 INOR **1511.** CO_2 capture enhancement in InOF-1 *via* the bottleneck effect of confined ethanol. **I. Ibarra**

4:25 INOR **1512.** Water stable Metal-Organic Frameworks (MOFs) for CO_2 capture. **D. Zhao**

4:45 INOR **1513.** Cooperative, adsorbate-induced spin transitions for efficient carbon monoxide separations in an Fe(II) metal–organic framework. **D. Reed**, B. Keitz, J.R. Long

5:05 INOR **1514.** Trapping gases in metal organic frameworks with a selective surface molecular barrier layer. **K. Tan**, S. Zuluaga, E. Fuentes, E. Mattson, H. Wang, J. Li, T. Thonhauser, Y.J. Chabal

5:25 INOR **1515.** Increased CO_2 adsorption in heterobimetallic MOFs obtained by post-synthetic transmetalations of HKUST-1. **J.M. Veleta**, R. Arrieta, M. Baeza, E. Barajas, K. Castañeda, C. Castañon, Z. Garcia, D. Villagran

Section G

Moscone Center

2024

Chemistry of Materials: Nanomaterials

C. G. Lugmair, *Organizer*

S. M. Noimark, L. J. Treadwell, *Presiding*

1:30 INOR **1516.** Dimerization of organic dyes on luminescent gold nanoparticles for ratiometric pH sensing. **S. Sun**, X. Ning, J. Zheng

1:50 INOR **1517.** Molecular layer deposition of ultrathin manganese oxide hybrid materials for catalysis applications. **D.S. Bergsman**, J.G. Baker, N. Yang, C. MacIsaac, A. Strickler, M. Lillethorup, S.F. Bent

2:10 INOR **1518.** Application of chiral tetrahexahedral Au nanoparticles in enantiomeric separations of chiral drugs. **N. Shukla**, D. Yang, Y. Zhao, A.J. Gellman

2:30 INOR **1519.** Synthesis and characterization of hollow Mn_3O_4 nanoparticles as anode materials for lithium ion batteries. **S. Varapragasam**, C. Balasanthiran, A. Gurung, Q. Qiao, R.M. Rioux, J.D. Hoefelmeyer

2:50 INOR **1520.** Multi-walled carbon nanotube-polymer composite coatings for optical ultrasound generation. **S.M. Noimark**, R. Colchester, S. Ourselin, I. Papakonstantinou, I.P. Parkin, A. Desjardins

3:10 Intermission.

3:25 INOR **1521.** Synthesis of N, P co-doped amorphous carbon dots and their toxicological impact on *Shewanella oneidensis* MR-1 bacteria. **B. Zhi**, M.J. Gallagher, B.P. Frank, T. Curry, T.A. Qiu, A.C. Mensch, Z. Rosenzweig, H. Fairbrother, R.J. Hamers, C.L. Haynes

3:45 INOR **1522.** Synthesis of nanoinks using novel precursors for advanced Direct Write applications. **L.J. Treadwell**, T.J. Boyle, N.S. Bell, A. Cook, D. Woodard, M.V. Parkes

4:05 INOR **1523.** Biocompatible and water-soluble gold-carbon nanoparticles. B. Atallah, I. Shehadi, M. Naggar, **A. Mohamed**

4:25 INOR **1524.** Surface functionalized metal-oxo polymer nanobeads as potential T_1 MRI contrast agents with dual reporting capability and specific targeting. **V. Dahanayake**, W.J. Hickling, O. Rodriguez, C. Albanese, S.L. Stoll

4:45 INOR **1525.** Investigation of nanosized metal oxides for thermal water splitting at reduced temperatures. **G. Larsen**, K. Coopersmith Lawrence, S. Hunyadi Murph

5:05 INOR **1526.** Cell-based targeted delivery of mesoporous silica nanoparticles loaded with a T1-contrast agent to 4T1 tumors. **H. Wang**, T.B. Shrestha, J. Covarrubias, A.P. Malalasekera, S.O. Wendel, J. Yu, P. Thapa, M. Pyle, D.L. Troyer, S.H. Bossmann

Section H

Moscone Center

3000

Chemistry of Materials: Materials for Energy & Catalytic Applications

C. G. Lugmair, *Organizer*

V. Doan-Nguyen, J. L. White, *Presiding*

1:30 INOR **1527.** Utilization of magnesium silicide as a reactive precursor for the facile synthesis of Si@Ge and Si@C composite electrodes for lithium-ion batteries. J. Ahn, M. Kang, D. Lee, H. Kim, Y. Sung, **W. Yoo**

1:50 INOR **1528.** Investigation of the reversible lithium insertion into anti-NASICON $Fe_2(WO_4)_3$. **G. Barim**, B.C. Melot, R.L. Brutchey

2:10 INOR **1529.** Transition metal polysulfide chalcogels as electrode materials for Li-ion batteries. **V. Doan-Nguyen**, K. Subrahmanyam, M. Butala, J.A. Gerbec, S. Islam, K. Kanipe, C. Wilson, M. Balasubramanian, K. Wiaderek, O. Borkiewicz, K.W. Chapman, P. Chupas, M. Moskovits, B. Dunn, M.G. Kanatzidis, R. Seshadri

2:30 INOR **1530.** Effect of nanostructuring on hydrogen storage properties of complex metal hydrides confined inside nanoporous carbons. **J.L. White**, V. Stavila, B. Wood, T. Heo, L.E. Klebanoff, E. Majzoub, M. Allendorf

2:50 INOR **1531.** Manganese oxide nanomaterials for electrocatalysis and energy storage. **T.N. Lambert**, J.A. Vigil, J. Duay, M. Kelly

3:10 Intermission.

3:25 INOR **1532.** Nb_4N_5/Nb_2O_5-rGO composites as pseudocapacitive anode materials for high power lithium ion batteries. **Y. Yan**, C. Lai, S. Robbennolt, B. Dunn, S.H. Tolbert

3:45 INOR **1533.** Modelling La_2NiO_4 for solid oxide fuel cell cathode applications. **A.L. Gavin**, G.W. Watson

4:05 INOR **1534.** Mechanisms and motivations for superionic conductivity in polyborane solid electrolytes from *ab initio* molecular dynamics. **B. Wood**, J. Varley, K. Kweon, P. Shea, V. Stavila, T.J. Udovic

4:25 INOR **1535.** Thermodynamics and kinetics at interfaces of metal hydrides for hydrogen storage. **S. Kang**, T. Heo, P. Shea, K.G. Ray, T. Ogitsu, S. Bonev, B. Wood

Section I

Moscone Center

3010

Organometallic Chemistry: New Ligand Platforms

N. S. Radu, *Organizer*

D. R. Manke, M. P. Marshak, *Presiding*

1:30 INOR **1536.** Structure-activity relationship of ruthenium metathesis catalysts in ethenolysis of cyclic olefins. **P. Engl**, C. Santiago, A. Fedorov, C. Coperet, M.S. Sigman, A. Togni

1:50 INOR **1537.** Blue phosphorescent zwitterionic Ir(III) complexes featuring weakly coordinating ligands. **K. Kirlikovali**, J.C. Axtell, P.I. Djurovich, D. Jung, V. Nguyen, B. Munekiyo, A.T. Royappa, A.L. Rheingold, A.M. Spokoyny

2:10 INOR **1538.** Caviplexes: Metal-Organic platforms for supramolecular recognition. **A. Pöthig**, P.J. Altmann

2:30 INOR **1539.** Influence of the phenylazopyridine ligand on the reactivity and electronic structure of (cyclopentadienyl)cobalt complexes. **E. McLoughlin**, K.M. Waldie, R. Sarangi, R.M. Waymouth

2:50 INOR **1540.** Synthesis, structure and reactivity of homo- and heterobimetallic complexes. **A. Nicolay**, T.D. Tilley

3:10 INOR **1541.** Homoleptic organolanthanide compounds supported by a bis(dimethylsilyl)benzyl ligand. **K. Boteju**, A. Ellern, A.D. Sadow

3:30 INOR **1542.** *m*-Terphenyl substituted β-diketonate ligands support coordinatively unsaturated metals. **M.P. Marshak**, E.S. Akturk, R.N. Seals

3:50 INOR **1543.** Modular synthesis of tris(aryl)tren ligands and their reactivity. V. Mdluli, **D.R. Manke**

4:10 INOR **1544.** Probing the π-acceptor/σ-donor ratio of 2-isocyanoazulene ligands as possible rivals of polyfluorinated organic isocyanides. **M.D. Hart**, J.J. Meyers, T. Nakakita, Z. Wood, N. Gerasimchuk, M.V. Barybin

4:30 INOR **1545.** Studies of protonation preferences in bifunctional late-metal organometallics: Applications to heterolytic C-H activation. **E.B. Hulley**, W. Christman, T. Morrow, N. Arulsamy

4:50 INOR **1546.** Influence of fluorescent dye containing ligand scaffolds on metal complex reactivity. **Z.M. Heiden**, N.R. Treich

Section J

Moscone Center

3012

Organometallic Chemistry: Synthesis & Characterization-Late Transition Metals

N. S. Radu, *Organizer*

Z. Assefa, D. C. Lacy, *Presiding*

1:30 INOR **1547.** Chemistry of gold(III) pincer complexes: Structure and reactivity Au-H and Au-CO complexes. **M. Bochmann**, J. Fernandez-Cestau, A. Pintus, L. Rocchigiani, P. Budzelaar

1:50 INOR **1548.** Synthesis, x-ray crystallography, spectroscopic and cytotoxicity studies of Au(I) complexes of tris(4-methoxy-3,5-dimethylphenyl)phosphine (MDMPP), bis (2-methoxyphenyl) phosphine (MPP) and further structural studies on higher coordinate Au(I) phosphine complexes. **Z. Assefa**, K. Brown, G. Agebeworvi, M. Kanipes-Spinks, C. Rorie

2:10 INOR **1549.** Homo-and heterobimetallic dicarbene complexes featuring unsymmetrical bis-NHC ligand. **M. Böhmer**, E.F. Hahn

2:30 INOR **1550.** Synthesis and reactivity of Ir^{III} complexes bearing NHC/imidazolyl chelate ligands. **T. Tan**, E.F. Hahn

2:50 INOR **1551.** Reactivity and dynamics of unsaturated cobalt *m*-terphenyl isocyanide complexes. **C. Chan**, J.S. Figueroa

3:10 INOR **1552.** Synthesis and reactivity of pincer-supported cobalt complexes. **L.M. Guard**, D.E. Linn, D.M. Heinekey

3:30 INOR **1553.** Metal-metal bonds from halide-bridged group 11 metal cations. **J.P. Sadighi**, C.M. Sato, J. Bacsa

3:50 INOR **1554.** Splitting water with an organomanganese tetramer. **D.C. Lacy**

4:10 INOR **1555.** Active site installation on a low valent iron cluster. **M.J. Drance**, J.S. Figueroa

4:30 INOR **1556.** Bonding in group 8 silylene complexes. **P. Smith**, T.D. Tilley

4:50 INOR **1557.** Rhenium β-diketiminates: Chemistry at the oxo moiety and in low-valent terminal oxo complexes. **T.D. Lohrey**, R.G. Bergman, J. Arnold

5:10 INOR **1558.** Frustrated Lewis pairs as ligands for late-transition metal complexes: Probing interactions in the coordination sphere. **B.R. Nichols**, J.L. Petersen, B.V. Popp

Section K

Moscone Center

3001

Chemistry of Materials: Synthesis & Properties

C. G. Lugmair, *Organizer*

B. A. Kilos, L. Vilà Nadal, *Presiding*

1:30 INOR **1559.** Composition manipulation of germanium nanocrystals via microwave-assisted colloidal synthesis. **K. Tabatabaei**, S. Kauzlarich, B. Nolan, H. Lu, X. Zhang, R.L. Brutchey, K. van Benthem

1:50 INOR **1560.** Study of Pt(II) precursors for focused electron beam induced deposition of Pt nanostructures. **H. Lu**, J.A. Spencer, Y. Wu, H. Fairbrother, L. McElwee-White

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

2:10 INOR **1561.** Long route from hexagonal-$AMn^{3+}O_3$ to $AMn^{2+}O_{2.5}$. **M. Olivier**, T. Pussacq, M. Huvé, F. Tessier, H. Kabbour

2:30 INOR **1562.** Withdrawn.

2:50 INOR **1563.** Thermolytic molecular precursor methods to germanium-doped single-sites on silica. **J.P. Dombrowski**, T.D. Tilley, A.T. Bell

3:10 INOR **1564.** Beyond thioureas: Highly monodisperse CdS nanocrystal syntheses via thiocarbonates, thiocarbamates, and thioureas. **L. Hamachi**, I. Jen-La Plante, G. Cleveland, J.S. Owen

3:30 INOR **1565.** Withdrawn.

3:50 Intermission.

4:05 INOR **1566.** Simple method to predict the electronic spin configuration of Fe(II) tris-diimine complexes. H. Phan, J. Hrudka, **M. Shatruk**

4:25 INOR **1567.** Non-covalent interactions in superatomic crystals. **J.L. Shott**, M. Freeman, N. Saleh, D.S. Jones, C. Bejger

4:45 INOR **1568.** Water confinement properties of a metal-organic nanotube. **M. Payne**, A.S. Jayasinghe, D. Unruh, T. Forbes

5:05 INOR **1569.** Synthesis and characterization of magnesium oxychloride as a fire resistant construction material. **R.F. Gochez**, C.L. Kitchens

5:25 INOR **1570.** Industrial outlook on the development of cost effective SiO_2 mesoporous cellular foams technology. **B.A. Kilos**, A.M. Kelly-Rowley, S. Matteucci, C.L. Tway, K. Mabe, H. Clements

5:45 INOR **1571.** Centimeter-sized epitaxial h-BN as a flexible & transferrable template for heteroepitaxial growth of semiconductor thin films. **H. Oh**, K. Chung, J. Jo, Y. Tchoe, H. Yoon, H. Lee, S. Kim, M. Kim, B. Sohn, G. Yi

Section L

Moscone Center

3003

Nanoscience

B. G. Trewyn, *Organizer*

E. Johlin, *Presiding*

1:30 INOR **1572.** Monocrystalline nanopatterned films made by nanocube assembly and chemical welding. B. Sciacca, A. Berkhout, M. van Huis, B. Brenny, A. Polman, **E. Garnett**

1:50 INOR **1573.** Graphene oxide membranes with strong stability in aqueous solutions and controllable lamellar spacing. **J. Hu**, Y. Xi, Z. Liu, R. Xie, X. Ju, W. Wang, L. Chu

2:10 INOR **1574.** Photovoltage, effective bandgap and photochemical charge transfer in nanoscale transition metal (Cu, Fe, Mn, Ni) doped $SrTiO_3$ photocatalysts. **X. Ma**, F.E. Osterloh

2:30 INOR **1575.** Semiconductor nanocrystals with compact fluorinated shells. **P. Xia**, M.L. Tang

2:50 INOR **1576.** 3D Nanostructure imaging via multi-energy deconvolution SEM. **E. Johlin**, M. de Goede, B. Sciacca, F. Boughorbel, E. Garnett

3:10 INOR **1577.** Opportunities and limitations for nanoscale photovoltaics to surpass the Shockley-Queisser limit. **S.A. Mann**, R. Grote, R.M. Osgood, A. Alu, E. Garnett

3:30 Intermission.

3:40 INOR **1578.** Metal halide perovskite nanowire arrays for photodetection with significantly improved stability. **Z. Fan**, L. Gu, M. Tavakoli, A. Waleed

4:00 INOR **1579.** Exploring of the scope of polyarylboranes. **M.W. Lee**, T. Wang

4:20 INOR **1580.** Efficiency of magnetic induction heating for single crystal iron oxide nanoparticles. R.R. Shah, T.P. Davis, A.L. Paulson, C.S. Brazel, **D.E. Nikles**

4:40 INOR **1581.** Elucidation of synthesis and characterization of non-precious nanoscale mixed metal oxides for green chemistry catalysis. **A.M. York**, C.A. Cadigan, R.M. Richards

5:00 INOR **1582.** Carrier selective contacts for nanowire solar cells. **S. Oener**, A. Cavalli, J. Haverkort, E. Bakkers, E. Garnett

5:20 INOR **1583.** TERS: Nanoscale Raman characterization of 0-1-and 2D materials. **A. Krayev**, M. Chaigneau

MEDI

Division of Medicinal Chemistry

A. Stamford, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin (see *COMP*, Tue)

ACS Chemical Biology Award Symposium (see *BIOL*, Tue)

Chemical Biology: Enabling Drug Discovery (see *ORGN*, Wed)

SOCIAL EVENTS:

Poster Sessions & Socials, 7:00 PM: Sun, Wed

BUSINESS MEETINGS:

Business Meeting (Open), 5:30 PM: Sun

Executive Committee Meeting (Closed), 8:30 AM: Sun

Long-Range Planning Committee Meeting (Closed), 5:30 PM: Mon

SUNDAY MORNING

Section A

Moscone Center

3002/3004

Macrocycles & Cyclopeptides in Medicinal Chemistry

M. J. Blanco-Pillado, *Organizer*

M. Blanco, *Presiding*

9:00 Introductory Remarks.

9:05 MEDI **1.** Simple ADME rules for complex molecules and life beyond the rule of 5. **S. Lokey**

9:40 MEDI **2.** Discovery of oral and BBB permeable eribulin analogs by taking advantage of its macrocyclic properties. **W. Zheng**

10:15 MEDI **3.** Peptides as shuttles for drug delivery to the brain. **E. Giralt**

10:50 MEDI **4.** Macrocyclic peptides as potential treatments for pain and drug abuse. **J.V. Aldrich**, S. Senadheera, T.F. Murray, J.P. McLaughlin

11:25 MEDI **5.** Milla molecule inhibitors of IAP proteins. **Y. Zhang**

12:00 Concluding Remarks.

Section B

Moscone Center

3006/3008

General Orals

A. W. Stamford, *Organizer*

I. M. Bell, *Presiding*

8:30 MEDI **6.** Development of a potent and selective bromodomain chemical probe. **M. Moustakim**, P. Brennan, D. Dixon

8:50 MEDI **7.** Structure-based computer-aided IL-6/GP130 Protein-Protein Interaction (PPI) inhibitor design. **G. Shi**, L. Mao, V. Kumari, C. Li

9:10 MEDI **8.** Disclosure of a development candidate to treat severe acute pancreatitis through a drug discovery partnership between GlaxoSmithKline and the University of Edinburgh. **J. Liddle**

9:30 MEDI **9.** Expanding screening decks by innovative MCR scaffolds. **A. Doemling**, P. Patil, R. Madhavachary

9:50 MEDI **10.** Metamorphosis of paroxetine into a highly potent and selective GRK2 inhibitor via structure-based drug design. **H. Waldschmidt**, K. Homan, O. Cruz - Rodriguez, M. Cato, R. Bouley, M. Wilson, A. Cannavo, J. Song, J. Cheung, P. Kirchhoff, W. Koch, J. Tesmer, S.D. Larsen

10:10 MEDI **11.** Discovery of novel potent and selective agonists of the serotonin (5-HT) $5\text{-}HT_{2C}$ receptor as neurotherapeutics. **H. Mack**, G. Backfisch, G. Blaich, W.M. Braje, T. Erhard, A. Haupt, A. Kling, V. Lakics, J.J. Lynch, M. Mugnaini, F. Pohlki, A.L. Relo, K. Schaefer

10:30 MEDI **12.** Assessment of MCHr1 target engagement in the brain using PET imaging. **A. Johansson**, M. Antonsson, A. Hogner, M. Fredenwall, M. Hayes, P. Johnstrom, M. Schou

10:50 MEDI **13.** Redox-responsive hyaluronic acid-taxoid nanoconjugate for CD44-targeted cancer chemotherapy. **Y. Zhang**, I. Ojima

11:10 MEDI **14.** Targeting ubiquitin pathway enzymes for cancer immunotherapy. **J. Wu**, H. Wang, S. Kumar, F. Wang, I. Sokirniy, C. Riling, M. Mattern, J. Weinstock

11:30 MEDI **15.** Synthesis and biological profiling of 2-azabicyclo[2.1.1]hexane-based proline isosteres as antagonists of TRPA1 ion channel. **D. Shore**, M. Volgraf, B. Safina, V.A. Verma, E. Villemure, H. Chen, L. Wang, A.A. Estrada, J.P. Lyssikatos, A. Kolesnikov, S. Do, S. Shields

11:50 MEDI **16.** Cyclophilin D inhibitors rational and fragment based design: From 7 mM to 7 nM potency. **C. Jorand-Lebrun**, X. Jian, T. Johnson, U. Graedler, D. Schwarz, B. Leuthner, A. Marx, D. Roche, M. Gilardone, H. Lemoine, S. Kulkarni, F. Bernard

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

SUNDAY AFTERNOON

Section A

Moscone Center

3002/3004

General Orals

A. W. Stamford, *Organizer, Presiding*

1:30 MEDI **17.** Discovery of AZD9977: A non-steroidal mineralocorticoid modulator for treatment of diabetic kidney disease. **K.L. Granberg**, Z. Yuan, B. Lindmark, K. Edman, K. Bamberg, A. Hogner, J. Kajanus, M. Malmgren, C. Löfberg, A. Nordqvist, J.Å. Lindberg, J. Brånalt, G. OMahony, M. Kossenjans, D. Liu, A. Aagaard, M. Billger, S. Bäckström, P. Cornwall, H. Ericsson, F. Erlandsson, E.L. Hansson, A. Hayen, M. Hermansson, I. Ivarsson, R. Jansson Löfmark, U. Johansson, U. Karlsson, X. Li, G. Nikitidis, P. Nordberg, A. Nordin, B. Polentarutti, N. Selmi, A. Turner, L. William-Olsson, C.E. Wingolf, J. Hartleib

1:55 MEDI **18.** Discovery of BMS-962212 a highly potent, selective inhibitor of coagulation FXIa. **D. Pinto**, M.J. Orwat, L. Smith II, S. Shrivastava, M.L. Quan, P.Y. Lam, K. Rossi, A. Apedo, J. Bozarth, Y. Wu, J. Zheng, B. Xin, N. Toussaint, P. Stetsko, O. Gudmundsson, E. Crain, P. Wong, Z. Lou, T. Harper, S. Chacko, J. Myers, S. Sheriff, H. Zhang, X. Hou, A. Mathur, D. Seiffert, J. Luettgen, R.R. Wexler

2:20 MEDI **19.** Development of new therapies for asthma based on compounds that specifically target $GABA_A$ receptors in the lung. **L. Arnold**, G.S. Forkuo, N.Y. Yuan, R. Kodali, O.B. Yu, N.M. Zahn, R. Jahan, G. Li, M.R. Stephen, M. Guthrie, A.N. Nieman, M.M. Poe, G.T. Yocum, C.W. Emala, D.C. Stafford, D.A. Steeber, J.M. Cook

2:45 MEDI **20.** Discovery of AGN-241689: A potent, orally-acting CGRP receptor antagonist for migraine prophylaxis. **I.M. Bell**

3:10 MEDI **21.** Discovery of BMS-986142: A reversible inhibitor of Bruton's Tyrosine Kinase (BTK) conformationally constrained by two locked atropisomers. **S.H. Watterson**, G.V. De Lucca, Q. Shi, C.M. Langevine, D.G. Batt, Q. Liu, M. Beaudoin Bertrand, H. Gong, J. Dai, H. Yip, P. Li, D.Z. Sun, D. Wu, C. Wang, Y. Zhang, S.C. Traeger, M.A. Pattoli, S. Skala, L. Cheng, M.T. Obermeier, R. Vickery, L.N. Discenza, C.J. D'Arienzo, Y. Zhang, E. Heimrich, K. Gillooly, T.L. Taylor, C. Pulicicchio, K. Mcintyre, M.A. Galella, A.J. Tebben, J.K. Muckelbauer, C. Chang, L. Salter-Cid, J.C. Barrish, P.H. Carter, A. Fura, J. Burke, J.A. Tino

3:35 MEDI **22.** Hydrogen bond interaction geometries in protein-ligand complexes: From large-scale statistics to single cases. **E. Nittinger**, T. Inhester, G. Lange, R. Klein, M. Rarey

4:00 MEDI **23.** Discovery of selective SETD8 inhibitors via structure-based approach. **A. Ma**, W. Yu, K. Butler, F. Li, W. Tempel, N. Babault, P. Fabio, J. Shao, J. Wang, M. Luo, M. Vedadi, P. Brown, C.H. Arrowsmith, J. Jin

4:25 MEDI **24.** Discovery of a noncovalent, mutant-selective epidermal growth factor receptor inhibitor. **B.K. Chan**, E.J. Hanan, K. Bowman, M.C. Bryan, D. Burdick, E. Chan, Y. Chen, S. Clausen, T. Dela Vega, J. Dotson, C. Eigenbrot, R. Elliott, R. Heald, P. Jackson, J. Knight, H. La, M. Lainchbury, S. Malek, H.E. Purkey, G. Schaefer, S. Schmidt, E. Seward, S. Sideris, L. Shao, S. Wang, S. Yeap, I. Yen, C. Yu, T.P. Heffron

4:50 MEDI **25.** Discovery of 4-(((2R,3R)-1,3-dihydroxybutan-2-yl)amino)-6-phenylpyrrolo[1,2-b]pyridazine-3-carboxamide (BMT-1438), a potent JAK1/3 inhibitor and the use of a phosphate prodrug in demonstrating efficacy in a rheumatoid arthritis model. **S.H. Spergel**, M. Mertzman, J. Kempson, J. Guo, S.M. Stachura, L. Haque, J. Lippy, R. Zhang, M.A. Galella, S. Pitt, G. Shen, A. Fura, K. Gillooly, K. Mcintyre, V. Tang, J.S. Tokarski, J. Sack, J. Khan, P.H. Carter, J.C. Barrish, S. Nadler, L. Salter-Cid, G.L. Schieven, S. Wrobleski, W.J. Pitts

Section B

Moscone Center
3006/3008

Medicinal Chemists' Toolbox: Factors Influencing Oral Bioavailability & Case Studies

N. A. Meanwell, P. M. Scola, K. Yeung, *Organizers*, *Presiding*

2:00 Introductory Remarks.

2:05 MEDI **26.** Drug absorption and disposition influencing oral bioavailability: An industrial perspective and literature review. **C. Huang**

2:40 MEDI **27.** First-pass intestinal glucuronidation as a potential obstacle for oral absorption of small molecule drug candidates: When should we worry? **A.S. Kalgutkar**

3:15 MEDI **28.** Role of drug metabolizing enzymes in oral bioavailability. **C. Khojasteh**

3:50 MEDI **29.** Role of early solubility measurements in predicting bioavailability challenges and subsequent formulation strategies to enable compounds. **W.P. Wuelfing**

4:25 MEDI **30.** Mesenteric lymph: A conduit to enhanced oral bioavailability and immune cell targeting. **C. Porter**

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

SUNDAY EVENING

Section A

Moscone Center
West Hall

General Posters

A. W. Stamford, *Organizer*

7:00 - 9:00

MEDI **31.** Aminobenzimidazoles and structural isomers: Design, synthesis, pharmacological evaluation and computational studies of novel dual-acting butyrylcholinesterase inhibitors and *h*CB_2 receptor ligands for the treatment of Alzheimer's disease. **D. Dolles**, E. Sawatzky, J. Möller, M. Nabissi, A. Drakopoulos, A. Strasser, H. Wittmann, M. Lohse, M. Decker

MEDI **32.** Development of small molecules to modulate Apoe and Abca1/Ldlr levels for Alzheimer's therapy. **N. John**, I. Boginski, A. Voigt, R. Remotigue, J. Kim, J. Kim, S. Maitra

MEDI **33.** Design, synthesis and biological evaluation of 3-hydroxy-4H-pyranone derivatives as potent MTDLs for Alzheimer's disease. **R. Sheng**, J. Liu, L. Jiang, L. Tang

MEDI **34.** Acetyl cholinesterase inhibitory and toxicity profiles of tacrine-curcumin hybrids. **R. Alavala**, G. Tipparapu, **S. Boyapati**, U. Kulanthaivelu, R. Ajmeera, B. Mantriprgada

MEDI **35.** Design, synthesis, and in vitro evaluation of novel sigma-2 receptor modulators: An opportunity in Alzheimer's disease therapy. **K. Blattner**, D.J. Canney, R. Gao, R. Bhandare, J.C. Gordon, M. Abou-Gharbia, N.J. Izzo, N. Knezovich, C. Silky, K. Mozzoni, S. Catalano, G. Rishton, B.E. Blass

MEDI **36.** Discovery of multi-target-directed ligands for the treatment of Alzheimer's disease. **W. Huang**, Z. Shen, C. Li, Q. Li, X. Zhen, Z. Ma, M. Liang

MEDI **37.** Biased agonism at CB2 cannabinoid receptors: Implications for drug development. **R. Hutchison**, P. Prather

MEDI **38.** Synthesis and biological evaluation of dual-target peripheral CB_1R antagonists. **M.R. Iyer**, R. Cinar, A.R. Katz, G. Kunos

MEDI **39.** Profiling signaling bias of synthetic cannabinoid New Psychoactive Substances (NPS) at the Cannabinoid Type 1 Receptor (CB1R). **S. Banister**, K.K. Kumar, B.K. Kobilka, S.V. Malhotra

MEDI **40.** Synthesis and SAR studies of somatostatin subtype-4 agonists for the treatment of Alzheimer's disease. **M. Minaeian**, A.M. Crider, I. Daryaei, M. Kontoyianni, W.M. Kolling, W.L. Neumann

MEDI **41.** Discovery of tetrahydroquinoline-containing CXCR4 antagonists with improved ADMET properties. **E.J. Miller**, E. Jecs, V. Truax, B. Katzman, K. Kuo, M.B. Kim, R.J. Wilson, H.H. Nguyen, Y.A. Tahirovic, M. Saindane, T. Wang, C. Sum, J. Chen, M.E. Cvijic, D.R. Shen, N. Burford, C. Chen, H. Zhang, A.J. Tebben, L.J. Wilson, G.M. Schroeder, D. Liotta

MEDI **42.** Synthesis of novel TIQ-15 analogs with improved drug properties. **E. Jecs**, E.J. Miller, R.J. Wilson, H.H. Nguyen, Y.A. Tahirovic, M.B. Kim, B.M. Katzman, V.T. Truax, K. Kuo, J. Chen, M. Cvijic, D.R. Shen, C. Chen, H. Zhang, A.J. Tebben, C. Sum, T. Wang, N. Burford, G.M. Schroeder, L.J. Wilson, D. Liotta

MEDI **43.** Synthesis and SAR of TIQ-15 based CXCR4 antagonists: Identification of tetrahydroquinoline replacements. **R.J. Wilson**, E.J. Miller, E. Jecs, V.T. Truax, L.J. Wilson, H.H. Nguyen, Y.A. Tahirovic, D. Liotta, G.M. Schroeder, T. Wang, H. Zhang, M. Kim

MEDI **44.** Synthesis of 2,4,6-trisubstituted pyridines using palladium-catalyzed cross-coupling reactions and in vitro anticancer evaluation. **A. Hernandez Campos**, P.J. Trejo, I. González, L. Yépez-Mulia, J. Pérez-Villanueva, M.A. Cerbón-Cervantes, R. Castillo-Bocanegra

MEDI **45.** First steps in hit-to-lead optimization towards AKT inhibition. **E.E. Sanabria-Chanaga**, R. Castillo-Bocanegra, A. Hernandez Campos

MEDI **46.** Design, synthesis and biological evaluation of quinazoline derivatives as cytotoxic molecules of breast cancer triple-negative. **A.S. Matus-Meza**, F. Hernández-Luis, M.A. Velasco-Velázquez

MEDI **47.** Targeting specific interactions to improve EGFR-ligand binding. C. Williams, A. Ajamian, N. Thorsteinson, **N. Li**, B. Jean-Claude

MEDI **48.** Molecular design and synthesis of inhibitors of EGFR kinase: New quinazoline derivatives. A.S. Bunev, E.V. Sukhonosova, **S. Sokov**

MEDI **49.** Derivatives of 5-(imidazo[2,1-*b*]thiazol-6-yl)-4-methylthiazol-2-amine new effective EGFR-kinase inhibitors. A.S. Bunev, E.V. Sukhonosova, **K. Talina**

MEDI **50.** Discovery of atropisomeric quinolinone sulfonamide (AM-0466), a potent and selective Na_v1.7 inhibitor with robust *in vivo* analgesic activity. **R. Graceffa**

MEDI **51.** Discovery of non-zwitterionic aryl sulfonamides as Na_v1.7 inhibitors with efficacy on preclinical behavioral and translational measures of pain. **Y. Wu**, J. Guernon, A. McClure, G. Luo, R. Rajamani, A. Ng, A. Easton, A. Newton, C. Bourin, D. Parker, K. Mosure, O. Barnaby, M. Soars, R.J. Knox, M. Matchett, R. Pieschl, J. Herrington, P. Chen, D. Sivarao, L.J. Bristow, N.A. Meanwell, J.J. Bronson, R.E. Olson, L.A. Thompson, C.D. Dzierba

MEDI **52.** Synthesis and structure-activity relationships of morpholine-based aryl sulfonamide Na_v1.7 inhibitors. **J.M. Guernon**, A. McClure, R. Rajamani, R.J. Knox, M. Matchett, R. Pieschl, J. Herrington, L.J. Bristow, N.A. Meanwell, R.E. Olson, L.A. Thompson, C.D. Dzierba, Y. Wu

MEDI **53.** Structure-based design of ATP citrate lyase inhibitors and their anticancer activities. F.E. Jernigan, S.K. Koerner, J. Hanai, V.P. Sukhatme, **L. Sun**

MEDI **54.** Withdrawn.

MEDI **55.** Bioassay protocols: Semantic annotation to enable informatics. **A. Clark**

MEDI **56.** Design, synthesis, and evaluation of a new privileged scaffold for use in drug discovery. **M.J. Stocks**, C. Schwehm, B. Kellam, A. Garces, N. Kindon, T. Bradshaw, J. Li, S.J. MacDonald, J. Rowedder

MEDI **57.** From chemical similarity to rational polypharmacology. **M.J. O'Meara**, X. Huang, B.L. Roth, B. Shoichet

MEDI **58.** Quantum chemistry calculation-aided optimization of novel microtubule-targeting agents binding to colchicine site. **C. Zheng**, J. Jiang, J. Liu, J. Zhu, Y. Zhou

MEDI **59.** Enhanced delivery of HIV integrase inhibitors with prodrugs designed for polymeric nanocarriers. **W.E. Afunugo**, M.E. Ebner, A.M. Bever, S. Cao, Y. Jiang, K.A. Woodrow, I.T. Suydam

MEDI **60.** Synthesis and biological evaluation of sulfonyl piperazine derivatives for LpxH inhibition. **M. Lee**, J. Zhao, J. Cho, D. Kwon, P. Zhou, J. Hong

MEDI **61.** Creating new from clinical agents: Discovery of Combretastatin A-4 inspired heterocycles as antitubulin anticancer agents. **N. Hura**, S.K. Guchhait

MEDI **62.** Matching medium characterization for microwave brain stroke imaging. T. Yilmaz, G.A. Eken, E. Yildirim, **M.H. Acar**, I. Akduman

MEDI **63.** Synthesis of functionalized benzofulvenes and their possible application towards thioredoxin reductase inhibition and cancer treatment. A. Glass, **K. Caspary**

MEDI **64.** Hologram QSAR and structure-based design of novel small-molecule inhibitors of choline acetyltransferase. **R. Kumar**, T. Darreh-Shori

MEDI **65.** Virtual hit-to-lead drug development program FRESH and success across carbonic anhydrase II and phosphatidylinositol 3-kinase α. **T. Kaiser**, Q. Shi, Z. Dentmon, P. Burger, J. Snyder, D. Liotta

MEDI **66.** Dopamine transporter ligands with short and long residence time. **S. Kukk**, J. Jarv

MEDI **67.** Structure function studies of silent agonists of the alpha 7 nicotinic acetylcholine receptor. **M. Quadri**, C. Stokes, R. Papke, C. Sanon, N. Horenstein

MEDI **68.** Dual soluble Epoxide Hydrolase (sEH) and Fatty Acid Amide Hydrolase (FAAH) inhibitors for treating. **S.D. Kodani**, K. Wagner, S. Hwang, K.S. Lee, C. Morisseau, B.D. Hammock

MEDI **69.** Low-cost high-impact route to kill MRSA with beta-lactam antibiotics. **C.V. Rice**, M. Foxley, M. Xiao, S. Wright, S. Strange

MEDI **70.** Clickable 4-*N*-alkanoyl and 4-*N*-alkylgemcitabine analogues with silicon-fluoride acceptors. **C. Gonzalez**, A. Sanchez, S.F. Wnuk

MEDI **71.** Novel 5-nitroimidazole and 5-nitrothiazole piperazine derivatives and their antiparasitic activity. **H.A. Saadeh**, M. Khasawneh, Y. Abou-Zeid, I. El-Haty, S. Nsangou, K. Goyal, R. Sehgal, A. Samadi

MEDI **72.** Matched molecular pair analysis and collaboration: Finding rules to the age-old problem. **A. Dossetter**, E.J. Griffen, A.G. Leach, S. Montague

MEDI **73.** Diketo acids and their hybrid bioisoster derivatives as bacterial biofilm and Methionine Aminopeptidase (MetAP) inhibitors. **A. Mohammad**, P. Hasan, V. Pillalamarry, M. Irfan, A. Perwez, B. Ahmad, U. Yadava, M. Rizvi, C. Daniliuc, R. Maguire, K. Kavanagh, A. Addlagatta

MEDI **74.** Studies aimed at the synthesis of Hsp90 inhibitors as antileishmaniasis agents. **L. Barbeto**, J. Leahy, D. Kyle

‡*Cooperative Cosponsorship*

MEDI **75.** Synthesis and biological activity studies of C1-substituted carbapenem antibiotics. **T. Nguyen**, J. Kim, P. Nguyen, M. Cox, M. Bennett, B. Meshram, L. Phung, C. Watanabe, A. Shi, M. Alqurafi, J.D. Buynak

MEDI **76.** 2-Nitrobenzenesulfonyl fluoride is a novel small molecule pharmacophore for the development of new antibiotics. **B. Park**

MEDI **77.** Gold-phosphines and gold-phosphine-modified human serum albumin as potent inhibitors of T-cell proliferation. **T.C. Dean**, M. Yang, M. Liu, P.K. Langston, J. Lee, C.M. Furdui, J. Grayson, U. Bierbach

MEDI **78.** Insulin: Its structure, function, and interaction in model cell membranes. **K. Saulcy**, D.C. Crans, A. Sostarecz

MEDI **79.** Synthetic and mechanistic studies of cyclotriazadisulfonamide (CADA) down-modulators of human CD4. **T.W. Bell**

MEDI **80.** Facile synthesis of Benzalkonium Chloride (BAC)-derived mesoporous silica nanoparticles as antibacterial material. **H. Wang**, T.B. Shrestha, J. Covarrubias, A.P. Malalasekera, S.O. Wendel, J. Yu, P. Thapa, L. Chlebanowski, O. Covarrubias Zambrano, D.L. Troyer, S.H. Bossmann

MEDI **81.** Withdrawn.

MEDI **82.** Advanced carbapenem antibiotics: The synthesis and activity studies of C6 substituted carbapenems. **M. Alqurafi**, J. Kim, D. Le, M. Lohry, C. Watanabe, A. Shi, T. Nguyen, J.D. Buynak

MEDI **83.** Impact of pH on solubility, hydrolysis kinetics, and pharmacokinetics of tenofovir disoproxil fumarate delivered from intravaginal rings. **J.A. Moss**, M.M. Baum, M. Gunawardana, C.S. Miller, I. Butkyavichene, S. Calvez, F. Yang, K.L. Vincent, R.B. Pyles

MEDI **84.** Withdrawn.

MEDI **85.** Use of substrate analogues and Tetrahydroisoquinolines (THIQ) as potential inhibitors for *Mycobacterium tuberculosis* enzyme MshC and synthesis of mycothiol. **K. Patel**, A. Reddy Maddirala, P.R. Andreana

MEDI **86.** MRI probe loaded HDL mimicking nanoparticles for diagnosis and therapy of atherosclerosis. **B. Banik**, S. Dhar

MEDI **87.** Copper responsive gadolinium-based MRI contrast agents. **N.N. Paranewithana**, A.F. Martins, G. Meloni, S. Chirayil, P. Zhao, A. Sherry

MEDI **88.** Novel, real-time analysis of nanomaterial inhibition of *E. coli*. **P.A. Sermon**

MEDI **89.** Organizing 3D project data for structure-based drug design. H.J. Feldman, A. Ajamian, **E. Metwally**

MEDI **90.** Fast generation of novel leads using virtual screening and fast MCR chemistry. **A. Doemling**, C.J. Camacho

MEDI **91.** Tumor suppressor $P27^{Kip1}$ regulation by tissue transglutaminase and its potential application in cancer therapeutics. **L. Zhang**, R.J. Sheaff

MEDI **92.** Withdrawn.

MEDI **93.** Dual targeting of the cancer antioxidant network with redox active gold(I) N-heterocyclic carbene complexes. R. McCall, J. Kocerha, J.L. Sessler, V. Sittaramane, K. Arumugam, **J.F. Arambula**

MEDI **94.** Fluorescent chemosensing for chloride and nucleotides based on artificial receptors in water. **A. Dorazco Gonzalez**

MEDI **95.** D-peptides as inhibitors of Proteinase 3-membrane interactions. K. Maximova, T. Venken, N. Reuter, **J. Trylska**

MEDI **96.** Molecular investigation of cyclic β- and γ-peptoids. **R. Grams**, D. Marron, M. Kassu, J.S. Josan

MEDI **97.** Mapping of cell surface receptors using silver nanodiscs. **J.S. Josan**, M. Kassu, G. Liu, A. Khan, R. Grams

MEDI **98.** Late-stage functionalization of complex molecules. **R. Karimov**, A. Sharma, J.F. Hartwig

MEDI **99.** Synthesis of novel imidazobenzodiazepine oxazole bioisosteres as potential alpha 2, 3 subtype selective GABA(A) receptors agonists with excellent metabolic stability, pharmacokinetics, and anxiolytic efficacy. **G. Li**, K.R. Methuku, M.M. Poe, J.M. Witkin, J.M. Schkeryantz, M. Ernst, J.M. Cook

MEDI **100.** Study and isolation of chemical compounds of *Guaiacum sanctum* for cytotoxicity and antitumor activities. **A.A. Laureano**

MEDI **101.** Synthesis and evaluation of increased binding affinity analogues of fosmidomycin as inhibitors of the non-mevalonate isoprenoid biosynthesis pathway. **B.C. Figula**, J.W. Tomsho, J.M. Gamrat

MEDI **102.** Design and synthesis of alpha-helix mimetics for treatment of high-risk human papillomavirus infection. **S. Rendon**

MEDI **103.** Design of ER beta selective agonists for hippocampal memory enhancements. **K. Perera**, W. Donaldson, A. Schulitz, D. Sem, J. Kim, K. Frick

MEDI **104.** Rational design, synthesis, and *in vitro* evaluation of mPGES-1 inhibitors as next-generation of anti-inflammatory drugs. **K. Ding**, Z. Zhou, Y. Yuan, F. Zheng, C. Zhan

MEDI **105.** Delivery of flavonol-based photoCORMs to mitochondria. **T. Soboleva**, H. Esquer, S. Anderson, A. Benninghoff, L.M. Berreau

MEDI **106.** Exploring the mechanism of action of a newly-discovered therapeutic peptide for blinding retinal diseases by identifying its receptors. **D. Zhou**, Z. Shao, J.A. Kornfield

MEDI **107.** Design of new irreversible arginase inhibitors. **X. Guo**, C. Seto

MEDI **108.** Development of biodegradable microneedles using dexamethasone and Poly Lactic-co-Glycolic Acid (PLGA) for cochlear drug delivery. **C. Bravo**

MEDI **109.** Alpha-helix mimetics as potential drugs for Human Papillomavirus (HPV). **V. Do**

MEDI **110.** Discovery of a novel irreversible and potent FLT3 inhibitor FF-10101 under clinical investigation. **M. Takasaki**, A. Hirai, D. Terada, M. Okubo, T. Tsujino, K. Sato, S. Tanabe, S. Inuki, S. Mizumoto, N. Fujikawa, D. Hirano, T. Yamaura

MEDI **111.** Discovery of CCT251236 from an HSF1 phenotypic screen: A pirin ligand with efficacy in an ovarian adenocarcinoma model. **E. Pasqua**, M. Cheeseman, N.E. Chessum, C. Rye, M.J. Tucker, B. Wilding, L.E. Evans, S. Lepri, M. Richards, S.Y. Sharp, S. Ali, M. Rowlands, L. O'Fee, A. Miah, A. Hayes, A.T. Henley, M. Powers, R. Te Poele, E. De Billy, L. Pellegrino, F. Raynaud, R. Burke, R.L. van Montfort, S.A. Eccles, P. Workman, K. Jones

MEDI **112.** Bruton's Tyrosine Kinase (BTK) program: Quick systematic SAR development utilizing parallel synthesis. Y. Yu, R. Anand, D. Sha, H.A. Vaccaro, M. Maletic, R. Mazzola, Z. Shi, M. Alhassan, S.B. Boga, J.L. Duffy, **X. Gao**, D. Guiadeen, J. Kelly, A. Krikorian, J. Liu, K. Maloney, O. Selytin, J. Wang, J. Xu, W. Yu, M. Altman, B.M. Andresen, Y. Liu, M. Martinez, T. Siu, S. Liu, C. Yang, H. Wu, J. Cai, Y. Gao, T. Fischmann, J. Presland, M. Mansueto, Z. Xu, E. Leccese, J. Zhang-Hoover, I. Knemeyer, C. Garlisi, N. Bays, P. Stivers, P. Brandish, A. Hicks, R. Kim, J.A. Kozlowski

MEDI **113.** Withdrawn.

MEDI **114.** Leucine's role of dry powder inhaler performance of salbutamol sulphate containing spray dried mannitol. **C. Molina**

MEDI **115.** Effects of varying H_2S concentrations on sulfhemoglobin complex formation. **N.E. Crespo Rosado**

MEDI **116.** Discovery of novel inhibitors of NF-kB Inducing Kinase (NIK) from an FBDD approach. **L. Kwok**

MEDI **117.** Utilizing the message-address concept to develop selective mu opioid receptor antagonists as potential treatment of opioid addiction. **S. Obeng**, A. Jali, D. Stevens, W.L. Dewey, D.E. Selley, Y. Zhang

MEDI **118.** Structure-activity relationships of phosphatidylinositol-3-kinase δ inhibitors for the treatment of inflammatory respiratory diseases. **A. Garces**, C. Schwehm, M.J. Stocks, N. Kindon, S.J. MacDonald, J. Rowedder, T. Bradshaw

MEDI **119.** Analysis of the binding parameters of the reversible inhibitor Argyrin B at the active sites of the constitutive and immunoproteasomes. D. Allardyce, C. Bell, **E. Loizidou**

MEDI **120.** Flavonol-based CO-releasing molecules: Tunability and albumin binding properties. **M. Popova**, T. Soboleva, L.M. Berreau

MEDI **121.** Identification of ligand-efficient inhibitors of *Trichomonas vaginalis* adenosine/guanosine preferring nucleoside ribohydrolase using NMR-based fragment screening. **S.N. Muellers**, A.L. Benzie, D.G. Brown, S. Cowen, D.W. Parkin, B.J. Stockman

MEDI **122.** Design, synthesis and employment of Flupirtine-derivative chemical probes for neuroprotective target identification. **N. Kinarivala**, F. Saadeh, J. Makoukji, R. Boustany, P.C. Trippier

MEDI **123.** Development of imidazopyridines and anti-proliferative effect against castration resistant prostate cancer cells. **I. Wazeerud-Din**, A. Millena, S. Khan, J. Bu

MEDI **124.** Novel chemotype of histone demethylase family KDM4 inhibitors. **M. Siklos**, M. Korczynska, T.A. Bates, B. Shoichet, D.G. Fujimori

MEDI **125.** Progress towards a novel class of immune modulators: Covalent toll-like receptor-7 agonists. **A.C. Chon**, A. Esser-Kahn

MEDI **126.** Novel prodrugs of transition state inhibitors of norovirus 3CL protease. **A. Galasiti Kankanamalage**, Y. Kim, K. Alliston, A.D. Rathnayake, M. Butler, S. Cardinale, T.L. Bowlin, K. Chang, W. Groutas

MEDI **127.** Cyclopropylthiazines as potent BACE1 inhibitors for Alzheimer's disease: Challenging chemistry and *in-vivo* data of this new pre-clinical series. **A. Siegmund**, K. Kong, M. Frohn, N. Nishimura, A. Pickrell, M.D. Bartberger, D. Hickman, J.R. Allen, S. Wood, M.P. Bourbeau

MEDI **128.** Threading the needle: Exploiting a P1-P3 ether linkage in the development of novel BACE inhibitors. **S.P. Walsh**, A. Shahripour, E. Kim, W. Li, J.D. Scott, D. Rindgen, L. Hyde, P. Orth, H. Wang, M. Kennedy, J. Cumming

MEDI **129.** Novel ROS activated prodrugs as kinase inhibitors: A strategy to improve selectivity. **P.N. Gurjar**, S. Abdul Salam, E.J. Merino

MEDI **130.** Design and synthesis of selective HADC6 inhibitors as potential agents against glioblastoma. **S. Fung**, A.A. Sadani, K. Wu, J. Chern

MEDI **131.** Solid-state structure and absolute configuration of enantiomers of 3-ethyl-3-phenylpyrrolidin-2-one. **A.V. Krivoshein**, S.V. Lindeman, V.N. Khrustalev, T.V. Timofeeva

MEDI **132.** Chemical correction of cellular dysfunction caused by progranulin deficiency in frontotemporal dementia. **M. Telpoukhovskaia**, K. Liu, C. Ludwig, J. Etchegaray, F. Sayed, Y. Zhou, M.S. Bogyo, S. Ding, L. Gan

MEDI **133.** Discovery and structure-activity relationship of thienopyridine derivatives as bone anabolic agent. **T. Shinozuka**, K. Saito, A. Nakao, K. Shimada, S. Matsui, N. Daisuke, N. Yoko, N. Satoru

MEDI **134.** Molecular modeling studies for a series of benzimidazole derivatives as cruzain inhibitors with anti-*Trypanosoma cruzi* activity. I. Pauli, **L. Ferreira**, M.L. de Souza, R. Ferreira, M. Dessoy, B. Slafer, G. Oliva, L.C. Dias, A.D. Andricopulo

MEDI **135.** Improving new molecule design using electrostatics. **T. Cheeseright**, M.D. Mackey

MEDI **136.** Structure-kinetics relationships for LpxC inhibition. **B. Lichtenthal**, C. Gu, F. Daryaee, R. Basu, M. Babar, P.J. Tonge

MEDI **137.** Problem based learning with MOE. **A. Bonin**

MEDI **138.** Exploiting solvent effects in drug design and optimization. R. Alvarez, A. Ajamian, **C. Williams**

MEDI **139.** Synthesis of novel efflux pump inhibitors which target the AcrAB-TolC multidrug efflux system in *Escherichia coli*. **K.M. Haynes**, N. Abdali, j. Parks, J.L. Chaney, A.T. Green, D. Wolloscheck, J.K. Walker, N. Wood, V.V. Rybenkov, J.Y. Baudry, J. Smith, H.I. Zgurskaya

MEDI **140.** Design of mGlu2 negative allosteric modulators for the treatment of neuropsychiatric disorders. **S. Conde**

MEDI **141.** Phosphonamidate inactivators of *Mycobacterium tuberculosis* (*Mtb*) *BlaC*. **D.S. White**, C. Choy, C.E. Berkman

MEDI **142.** Development of covalent caspase-6 inhibitors derived from disulfide trapping (tethering). **K.S. Van Horn**, D. Wang, C. Bryant, D. Medina-Cleghorn, P. Jaishankar, P. Lee, M. Arkin, A.R. Renslo

MEDI **143.** What do recently approved oral drugs look like? A year-by-year analysis of FDA approved drugs in 2007-2016. **A. Ritzén**, L. David

MEDI **144.** μCyclic peptides containing tryptophan and arginine residues: Antibacterial activities and structure-activity relationship. **N. Riahifard**, T. Aldakhil, S. Nasser, F. Nunez, K. Zoghebi, S. Mozaffari, J. Yamaki, K. Parang, R.K. Tiwari

MEDI **145.** Synthesis and evaluation of antimicrobial activity of levofloxacin-[R_4W_4] and Q-levofloxacin-[R_4W_4] conjugates and comparison with the corresponding physical mixtures. **N. Riahifard**, K. Tavakoli, J. Yamaki, R.K. Tiwari, K. Parang

MEDI **146.** Anti-malarials targeting the heat shock 90 protein of *Plasmodium falciparum*. **N. Everson**, J. Bach, T. Sisley, M. Walls, S.C. Eagon

MEDI **147.** Synthesis of anti-malarial compounds targeting the ATP4 protein in *Plasmodium falciparum*. G. Koch, J. Tryhorn, K. Ahn, B. Belanger, K. Yniguez, **H. Lazaro**, A. Kashtanova, S.C. Eagon

MEDI **148.** Novel high-affinity dopamine D4 receptor-selective ligands. **C.A. Boateng**, T.M. Keck, B. Free, C. Wu, A. Bonifazi, A.H. Newman, D.R. Sibley

MEDI **149.** Optimized chemical tools to probe the function of thioredoxin-interacting protein as therapeutic target. **O. Mirguet**, S. Nicolas, M. Aumis, K. Daeron-Courté, F. Perron-Sierra, S. Guizzetti, C. Vinson, A. Caliez, C. Chesneau, B. Cremers, M. Sadlo, I. Wehrle, G. Zanirato, P. Delerive, C. Bernard

MEDI **150.** Structure activity relationship of novel piperazino-enaminones (JOAB series) as pro-inflammatory cytokines suppressants. A. Bill, D. Szollosi, J. Dhuguru, I. Edafiogho, **O.M. Ghoneim**

MEDI **151.** Phytochemical evaluation of antimicrobial properties of *Combretum igneiflorum* extracts. **I. Maldonado**, A.K. Addo-Mensah

MEDI **152.** Next generation small molecule inhibitors of 5'-Methylthioadenosinenucleosidase (MTN) as novel antimicrobial agents. J.H. Thurston, K. Cornell, **L. Wayment**

MEDI **153.** Synthesis and evaluation of choline-derived Deep Eutectic Solvents (DES) as biofilm eradicating antibiotics. **A.W. Jemas**, D. Jacobs

MEDI **154.** Structure Activity Relationship (SAR) studies of EP2 receptor antagonists. **T. Ganesh**, R. Dingledine

MEDI **155.** Identification of vacuolar (H^+)-ATPase modulators by virtual screening process. R. Patil, A. Kulshrestha, A. Tikoo, S. Fleetwood, G. Katara, W. Seibel, A. Gilman-Sachs, **S. Patil**, K. Beaman

MEDI **156.** Identification of a novel chemotype of ASK1 inhibitors for heart failure utilizing structure-based drug design. **A.L. Chambers**

MEDI **157.** Determination of partition and distribution coefficients using ^{1}H NMR spectroscopy time domain Complete Reduction to Amplitude-Frequency Table (CRAFT) analysis. **D.P. Soulsby**, J. Chica

MEDI **158.** Synthesis, cytotoxic evaluation and docking studies of novel 9-anilinothiazolo[5,4-*b*]quinoline derivatives bearing polar groups at the anilino ring. **A. Lira-Rocha**, V. Tinajero-Delgado, **J. Solano-Becerra**

MEDI **159.** Identification of R419, an indirect AMPK activator. **S.J. Shaw**, D. Goff, D.C. Carroll, R. Singh, D. Sweeny, G. Park, D. Lau, Y. Jenkins, V. Markovtsov, T. Sun, Y. Li, A. Pan, Y. Hitoshi, K. Baltgalvis, H. Nguyen, T. Kinsella, D. Payan

MEDI **160.** Effects of propolis on cancer cell membranes and bacterial cell membranes studied with Langmuir monolayers. **B. Book**, A. Sostarecz

MEDI **161.** Langmuir monolayer investigation in to the antibacterial properties of essential oils. **A. Axup**, A. Sostarecz

MEDI **162.** Synthesis and antiproliferative activities of doxorubicin thiol conjugates and doxorubicin-S-S-cyclic peptide. **S. Darwish**, N. Sadeghiani, **R. Tiwari**, **K. Parang**

MEDI **163.** Radiosynthesis of $P2X_7$ receptor radioligands [^{11}C]GSK1482160 and [^{11}C] GSK1482160 isomer under different base conditions. **M. Gao**, M. Wang, Q. Zheng

MEDI **164.** Fully automated synthesis of [^{11}C]Me-GDC-0068 as a PET tracer for imaging of Akt in cancers. **M. Gao**, M. Wang, H. Shannon, B. Bailey, K. Pollok, H. Zarrinmayeh, Q. Zheng

MEDI **165.** Natural product-inspired agents and their anticancer activity against glioblastoma multiforme cells. **V. Kumar**, S. Banister, H. Hunter Kaufman, J. Vittimberga, S.A. Jacobo, S.S. Gambhir, S.V. Malhotra

MEDI **166.** CDD vault: A modern approach for drug research project team informatics. **W.W. Smith**, B.A. Bunin, K. Gregory

MEDI **167.** Novel tetrahydro isoquinoline derivatives as LXR modulators. **A. Chatterjee**, T.P. Burris, K. Griffett, S. Banerjee, Z. Doerer, A. Avdagic, T. Boehm, **J.K. Walker**

MEDI **168.** From photochemically responsive crystals to anticancer compounds: Discovery of novel anthracene analogs as antineoplastic agents. **I. Islam**, A. Nehdi, R.O. Al-Kaysi, A. Alaskar, M. Boudjelal

MEDI **169.** Design, synthesis, and biological properties of a fluorescent duocarmycin analog: HxTfA. K. Kiakos, P.C. Patil, S. Yanow, J.A. Hartley, **M. Lee**

MEDI **170.** Evaluated as potential hypocholesterolemic agent, the preparation and characterization of steroidal ∝,β-unsaturated ketones. E.J. Parish, **D. Ren**, Y. Lo, G. Ren, **H. Honda**

MEDI **171.** Novel approaches to the chemical preparation and characterization of kinsenoside. **D. Ren**, Y. Lo, E.J. Parish, **H. Honda**

MEDI **172.** New compounds for the treatment of *Mycobacterium abscessus* infections. **K.D. Combrink**, F. Maurer, K. Elizondo, A. Ramirez-Ramos, S. Spring

MEDI **173.** Anticancer activity of *exo*-cyclic carbohydrate enones containing thiophene and pyrolle moieties. J. Sarnik, A. Czubatka-Bienkowska, A. Macieja, **Z.J. Witczak**, R. Bielski, T. Poplawski

MEDI **174.** Novel carbohydrate functionalized thiosemicarbazides evoked DNA damage in cancer cell lines. A. Czubatka-Bienkowska, J. Sarnik, **Z.J. Witczak**, T. Poplawski

MEDI **175.** Enhanced chemical diversity through library *in situ* pre-metabolism: Using biological chemistry for novel lead discovery. N.J. Ayon, **W.G. Gutheil**

MEDI **176.** Actinomycete antibiotic compounds from soil bacteria at an ancient Roman site. **A. Hoffman**

MEDI **177.** Inhibitors of the protein-protein interaction of Class IIa HDACs with MEF2 as potential anticancer agents. **C.M. DeAngelo**, K.J. Gaffney, M.A. Sainz, J.A. Jarusiewicz, N. Jayathilaka, L. Chen, S.G. Louie, N.A. Petasis

MEDI **178.** Development and screening of new cathepsin B and K inhibitors utilizing substituted thiosemicarbazones. **R. McConnell**, H. Sarepalla, P.G. Akula, B. Guda, D. Yermala, N. Kadasala, K. Sayyar, W. Godwin, L. Wen

MEDI **179.** Novel mPGES-1 inhibitors identified from structure-based virtual screening based on new acting mechanism. **S. Zhou**, Z. Zhou, Y. Yuan, C. Zhan

MEDI **180.** Nanomolar-potency aminophenyl-1,3,5-triazine CFTR chloride channel activators for pro-secretory therapy of dry eye diseases. **S. Lee**, P. Phuan, C. Felix, M.H. Levin, A. Verkman

MEDI **181.** Development of novel anti-biofilm compounds for the prevention and treatment of Candidiasis. **M. Valdez**

MEDI **182.** Anti-bacterial activity of isoxazole rifamycin derivatives against *Mycobacterium abscessus*. **A. Ramirez Ramos**, K.D. Combrink, F. Maurer, S. Schmidl, S. Spring, K.N. Elizondo

MEDI **183.** Identical HIV populations and levels of proviral expression in lymph nodes and PBMCs in individuals on antiretroviral therapy. **V. Musick**

MEDI **184.** Synthesis and evaluation of 1, 3, 5 (10) estratriene aminoalkyloxy,16-formyl derivatives of Estrone as potential anti-breast cancer agents. **C. Sullen**, J.S. Cooperwood

MEDI **185.** Modulation of Glioblastoma tumor area is time dependent on the application of G4-OH PAMAM dendrimer. **M. Jeakle**

MEDI **186.** Polymorphs and solvates of erlotinib and dasatinib. **T. Maddox**, R. Quinones

MEDI **187.** Computer-aided design of negative allosteric modulators of metabotropic glutamate receptor 5 (mGluR5):CoMFA studies on aryl ether derivatives. S. Chelliah, **B. Jordan**, R. Thilagavathi

MEDI **188.** Chemo-enzymatic approach towards the synthesis of vancomycin and its analogs. **S. Ozturk**

MEDI **189.** EGCG and Sylibins as treatment for inherited cardiomyopathies: Binding simulations to cardiac troponin. **J. Eiros Zamora**, G. Hoben, A. Sheehan, A. Messer, A. Chaudhry, D. Biedermann, V. Kren, S.B. Marston, I.R. Gould

MEDI **190.** Derivatives of L-tryptophanhydroxamic acid as potential inhibitors of *Burkholderia pseudomallei* IspF. **C. Muller**

MEDI **191.** Synthesis and evaluation for biological activity of cyclic guanidine containing natural product analogues. **V. Sammeta**, **S. Rasapalli**

MEDI **192.** Exploring the chemical biology of secondary metabolites: Scalable synthesis of majusculamide D. **E.J. Caro-Diaz**, W.H. Gerwick

MEDI **193.** Prostate cancer targeted nanoparticle cocktail for combination therapy. **U. Basu**

MEDI **194.** Direct thrombin inhibitors with a novel, reversible, covalent mechanism of action. M. Sivaraja, S. Sizikov, D. Williams, C. Xu, D. Clemens, S. Dash, K. Lin, M. Reddy, G. Neckermann, S. Yau, E. To, L. Igoudin, S. Chang, S. Keutzer, P. Zalicki, N. Sandoval, J. Zhang, T. Shiau, **K. Short**, M. Estiarte, A. Datta, D. Kita

MEDI **195.** Cheminformatics analysis of WNK-inhibitor interactions. **M.A. Kuenemann**, D. Fourches

MEDI **196.** Computational structural-based design and structure and activity study of fluorinated combretastatin analogues. **Y. Zong**

MEDI **197.** Benzoate derived pH sensitive phosphoramidate-based linkers for controlled release. **B. Backer**, A. Davis, C. Choy, C.E. Berkman

MEDI **198.** New vacuolar-ATPase inhibitors as antiviral therapies. **A. Lindstrom**, D.P. Petrov, D. LaCount, R. Davey, V.J. Davisson

MEDI **199.** Design and synthesis of curcumin analogues for cytotoxicity against head & neck cancer. **S. Chelliah**, B. Jordan, B. Kumar, R. Thilagavathi, P. Kumar

MEDI **200.** Withdrawn.

MEDI **201.** Interactions of isoniazid with model membranes. **A. Groninger**, B.J. Peters, J.B. Hough, F. Fontes, G. Cardiff, D.C. Crick, D.C. Crans

MEDI **202.** Synthesis and biological evaluation of novel casein kinase 1d inhibitors for treatment of Alzheimer's disease. **V. Jha**, C. Gettridge, R. Schroeder, M. Bratton, P. Tram, J. Sridhar

MEDI **203.** Exploring the interactions between the anti-tuberculosis agent, pyrazinamide/pyrazonoic acid, and lipid model membrane systems. **J.B. Hough**, A.S. Groninger, B.J. Peters, F. Fontes, D.C. Crick, D.C. Crans

MEDI **204.** Aza-peptide aldehydes and ketones: A new class of proteasome inhibitors. **T. Corrigan**, K. Kasper, R. McCauslin, R.J. Yoder, C.M. Hadad, Ö. Doğan Ekici

MEDI **205.** Synthesis of oligothiophene tris(2,2'-bipyridyl)-type ruthenium (II) conjugate as electrochemiluminescence-luminophore. **L. Lantz**, P. Nilsson

MEDI **206.** Molecular dynamic simulation and pharmacophore model of parasitic cysteine proteases. **D. Gomes Vital Fujii**, **G.M. Monteiro Ferreira**, **J. da Fonseca Rezende e Mello**, **G.H. Trossini**

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MEDI **207.** Comparison of the efficacy of ester substituents in their specificity and effectiveness for reducing cell growth in certain cancer cell lines. **R. Nguyen**, A. Jelowicki, M. Young, C. Bunye, K. Soriano, E. Guglielmo, E. Lavassani, A. Nguyen, N. Patel, P. De Lijser

MEDI **208.** Synthesis of KS15 derivatives as CRY-mediated circadian clock modulators. **Y. Choi**, Y. Son, S. Chung, G. Son, K. Kim, Y. Suh, J. Jung

MEDI **209.** Synthesis and evaluation of xanthurenic acid analogs for impeding transmission of *Plasmodium falciparum* from host to vector. **A. Kanwar**, J. Leahy, D. Kyle, T. Mcgaha

MEDI **210.** Withdrawn.

MEDI **211.** Magnetite nanoparticles effect on *Escherichia coli* growth. **M.A. Gratacos**, E. Acevedo

MEDI **212.** Withdrawn.

MEDI **213.** Developing dual colorimetric and fluorogenic probes for visualizing tyrosine phosphatase activity and high throughput screening. **S. Biswas**, B. S. McCullough, E. S. Ma, D. LaJoie, C. W. Russell, G. Brown, J. L. Round, K. S. Ullman, M. A. Mulvey, A.M. Barrios

MEDI **214.** Photoswitchable dualsteric M1 ligand. **L. Agnetta**, M. Kauk, M. Canizal, R. Messerer, U. Holzgrabe, C. Hoffmann, M. Decker

MEDI **215.** Synthesis of chemical probes for serine/threonine protein phosphatase 5C based on a natural product template. **M. Tuttle**, L. Yet, R. Honkanen, M. Swingle

MEDI **216.** Development and synthesis of β-lactam prodrugs for tuberculosis. **M. Cole**, J. Buonomo, C.C. Aldrich

MEDI **217.** Synthesis and biological evaluation of a novel series of GPER antagonists for the treatment of gallstone formation. **C. DeLeon**, C.K. Arnatt, D. Wang, M. Wilhelm, P. Sweeney

MEDI **218.** Design, synthesis and SAR study of truxillic acid-based fatty acid binding protein inhibitors as anti-nociceptive and anti-inflammatory drugs. **S. Yan**, K. Hu, S. Tong, M. Awwa, Q. Gan, M. Elmes, J. Sweeney, H. Hsu, M. Kaczocha, H. Li, R.C. Rizzo, D. Deutsch, I. Ojima

MEDI **219.** SB-T-1214 and biotin functionalized gold nanoparticles. **X. Wang**, I. Ojima

MEDI **220.** Discovery of a novel series of potent and selective Phosphatidylinositol-3-Kinase delta (PI3Kδ) inhibitors for the treatment of inflammatory and autoimmune diseases. **N. Aguilar**, J. Fernandez, B. Hernandez, M. Carrascal, P. Niño, A. Lopez, L. Vazquez, E. Lozoya, M. Maldonado

MEDI **221.** Development of cancer stem cell depleting ALDH1A selective inhibitors as potential therapeutics for ovarian cancer. **B. Huddle**, C. Buchman, K. Yang, M. Chtcherbinine, I. Chefetz-Menaker, C. Morgan, R. Buckanovich, T. Hurley, S. Larsen

MEDI **222.** Photoaffinity probes for protein N-terminal methyltransferases. **B. Mackie**, R. Huang

MEDI **223.** Novel selenorhodamine dyes as photosensitizers in varying applications. **J. Hill**, M.W. Kryman, G.A. Schamerhorn, M.R. Detty, Z.A. McIver

MEDI **224.** Design, synthesis and preclinical study of novel taxoid-based Small Molecule Drug Conjugates (SMDCs) using folate/Dimethyltetrahydrofolate (DMTHF) as tumor targeting module. **C. Wang**, Y. Wang, M. Tortorella, I. Ojima

MEDI **225.** Structure-based discovery of novel small molecule Wnt/β-catenin signaling inhibitors. **S. Guzman**, A. Nguyen, P. De Lijser, N. Patel

MEDI **226.** Identification and lead optimization of pyrazole carboxamides with antiviral activity. **K. Paulvannan**

MEDI **227.** Inhibition of arginase from *Leishmania mexicana* by benzimidazole derivatives. **I. Betancourt**, A. Chaidez-Avila, A.G. Vazquez-Raygoza, C.I. Avitia-Domínguez, A. Romo-Mancillas, A. Hernandez Campos, A. Téllez-Valencia

MEDI **228.** Design and development of a novel class of structurally-enhanced allosteric modulators of hemoglobin for sickle cell disease treatment. **P. Pagare**, O. Abdulmalik, M.K. Safo, Y. Zhang

MEDI **229.** Generation of novel leads for γ-secretase modulation. **M. Mandal**

MEDI **230.** Synthesis of benzimidazole derivatives for uridine nucleoside ribohydrolase targeting. **A.S. Leonardo**, M.A. Vanalstine-Parris

MEDI **231.** Synthesis and biological evaluation of the first triple inhibitors of human topoisomerase 1, tyrosyl-DNA phosphodiesterase 1 (Tdp1), and tyrosyl-DNA phosphodiesterase 2 (Tdp2). P. Wang, **M.S. Elsayed**, C. Plescia, E. Kiselev, C. Marchand, O. Zeleznik, K. Agama, Y. Pommier, M. Cushman

MEDI **232.** Transcarbamoylation of sulfonyl carbamates to generate new Angiotensin II Type 2 Receptor (AT2R) ligands. J. Wannberg, **R. Isaksson**, M. Hallberg, M. Larhed

MEDI **233.** Development of new novel therapeutics for refractive breast cancer. **K. Crosby**, **K. Johnson**

MEDI **234.** Design, synthesis and pharmacological evaluation of 1,3,6-trisubstituted-4-oxo-1,4-dihydroquinoline-2-carboxylic acid derivatives as selective ET_A antagonists. **N.S. Khadtare**, R. Stephani, V.L. Korlipara

MEDI **235.** Withdrawn.

MEDI **236.** Structure-based design of small-molecular inhibitors targeting the Menin-MLL protein-protein interaction. **S. Xu**, T. Xu, K. Zheng, A. Aguilar, L. Huang, D. Bernard, D. McEachern, S. Przybranowski, J. Stuckey, S. Wang

MEDI **237.** Novel pirfenidone derivatives: Potent antifibrotic agents. **Z. Ma**, C. Yu, Q. Chen, W. Huang, Z. Wang, C. Zhang, Z. Shen

MEDI **238.** Synthesis and biological activity of novel TU-100 derivatives. **O.J. Alao**, R.J. Sheaff, J.C. Dicesare

MEDI **239.** New α-helix mimetics targeting the E6 protein in the human papillomavirus. **E. Armenta**, A. Orchard

MEDI **240.** Finding hits for designing new antidiabetic drugs. Inhibition of protein tyrosine phosphatase 1B. M.J. Sarabia-Sánchez, P.J. Trejo, E. Sierra, M. Valdez-Solana, A. Hernandez Campos, C.I. Avitia-Domínguez, **A. Téllez-Valencia**

MEDI **241.** Identification of small molecular activators on the unfolded protein response in leukemia cells. **N. Mahmoud**, D. Garshott, Y. Xi, A. Brownell, M. Callaghan, A. Fribley

MEDI **242.** Constrained peptides that inhibit HIV-1 fusion. **O. Bolarinwa**, J. Cai

MEDI **243.** Design and optimization of small molecule inhibitors blocking the menin-MLL interaction. **T. Xu**, S. Xu, K. Zheng, A. Aguilar, L. Huang, K. Chinnaswamy, D. Bernard, D. McEachern, S. Przybranowski, J. Stuckey, S. Wang

MEDI **244.** Discovery of LLM4 as potent and specific IL-6/gp130 protein-protein interaction inhibitor for potential cancer therapy. **L. Mao**, G. Shi, C. Li

MEDI **245.** ML418: The first selective, sub-micromolar pore blocker of $K_v7.1$ potassium channels. **H. Kurata**, D.R. Swale, S.V. Kharade, J. Sheehan, R. Raphemot, K.R. Voigtritter, E.E. Figueroa, J. Meiler, A.L. Blobaum, C.W. Lindsley, J.S. Denton, C.R. Hopkins

MEDI **246.** Effect of magnetite chitosan/alginate beads infused with the antibiotic oxytetracycline hydrochloride on *E. coli* growth rates. **R.M. Zamora**, A. Chardon, F. Alvarez, A. Zapata, V. Fernandez-Alos, F. Roman, O. Perales

MEDI **247.** Design and solid-phase synthesis of Muramyl dipeptide (MDP) surrogates as NOD2 signaling activating agents. **I. Kekessie**, T. Goncharov, J. Tom, D. Vucic, A. Song

MEDI **248.** Discovery of preclinical candidate SCH 900577: A prodrug of hydantoin based TACE inhibitor. **L. Tong**, S. Kim, L. Chen, A. Kosinski, B. Shankar, V. Girijavallabhan, D. Yang, W. Yu, G. Zhou, N. Shih, K. Rosner, D. Li, C. Dai, J. Popovici-Muller, L. Yang, A. Siddiqui, Z. Guo, P. Orth, S. Chen, M. Hu, D. Lundell, X. Niu, S. Umland, J.A. Kozlowski

MEDI **249.** Probing conformational preference: (S)- and (N)-methanocarba 7-deazaadenosine analogues as inhibitors of human adenosine kinase. **K.S. Toti**, D. Osborne, A. Ciancetta, D. Boison, K.A. Jacobson

MEDI **250.** Synthesis and NMDA receptor activity of various ketamine metabolites. **P.J. Morris**, P. Zanos, R. Moadell, C.A. Zarate, T. Gould, C.J. Thomas

MEDI **251.** Discovery of potent glucagon receptor antagonists for the treatment of type 2 diabetes. **G. Xu**, M.D. Gaul, F. Song, B. Zhao, Y. Liang, F. Du, K. Diloreto, N. Huebert, B.C. Shook, D. Rentzeperis, R. Santulli, A. Eckardt, C. Smith, K. Demarest

MEDI **252.** Synthesis and two- and three-dimensional *in vitro* studies of hyaluronic acid porphyrin conjugates. **N. Bhupathiraju**, C. Farley, N. Berisha, B. Begum, C.M. Drain

MEDI **253.** Preformulation analysis and stability of hydrophobic small molecular echinomycin for injection formulation. **J.H. Lee**, M. Tran, P. Yuan, G.K. Potti

MEDI **254.** Withdrawn.

MEDI **255.** Design, synthesis and biological evaluation of specific ARK5 inhibitor. **M. Reddy**, S. Athuluri-Divakar, B. Akula, M.R. Mallireddigari, S.C. Cosenza, V. Dandu, V. Bharathi, V. Pallela, P. Reddy

MEDI **256.** Discovery of novel class IIa-selective histone deacetylase inhibitors using an in silico virtual screening approach. **H. Tseng**, C. Liu, C. Chen, K. Hsu, W. Huang

MEDI **257.** Hybridization approach to selective RIPK2 inhibitors by targeting inactive kinase conformations. **C. Suebsuwong**, A. Degterev, G. Cuny

MEDI **258.** Design and synthesis of tricyclic and tetracyclic fused coumarin sulfonate derivatives, and their inhibitory effects on LPS-induced nitric oxide and PGE_2 productions in RAW 264.7 macrophages. **M.I. El-Gamal**, C. Oh, K. Lee, D. Baek

MEDI **259.** Novel benzamides as capsid assembly modulators for the hepatitis B virus. **N. Hwang**, M. Campagna, K. McGuire, S. Wu, J. Guo, Y. Du

MEDI **260.** Computational design, synthesis and characterization of novel mPGES-1 inhibitors. **Z. Zhou**, K. Ding, S. Zhou, Y. Yuan, F. Zheng, C. Zhan

MEDI **261.** Evaluation of 2-amino-pyrimidine derivatives as antimicrobial agents and IspF inhibitors. **S. Watkins**, D. Ghose, C.A. Muller, Z. Zhang, J.M. Blain, Z. Lazowski, S.T. McDonald, T. Riggins-Walker, J.R. Horn, R. Meganathan, H. Hofstetter, T.J. Hagen

MEDI **262.** Design and synthesis of 1-(2-(2,4-difluorophenyl)-2-hydroxy-3-(1H-1,2,4-triazol-1-yl)propyl)-2-(1-((methyl(3-(((methylcarbamoyl)oxy)methyl)pyridin-2-yl)carbamoyl)oxy)ethyl)-1H-1,2,4-triazol-2-ium. **L. Peyton**, M. Hashemzadeh, S. Gallagher

MEDI **263.** Fragment-based lead discovery of a novel Map4k4 inhibitor. **L. Wang**

MEDI **264.** SDAP substrate analog enantioselective synthesis and ninhydrin-based enzyme assay for the dapE-encoded bacterial enzyme diaminopimelate desuccinylase (DapE). **T. Heath**, M. Lutz, C. Reidl, B. Nocek, M. Ballicora, R.C. Holz, K. Olsen, D.P. Becker

MEDI **265.** Discovery of a new class of highly potent small-molecule degraders of BET bromodomain proteins. **F. Xu**, J. Hu, B. Zhou, Z. Chen, M. Lin, L. Bai, C.Y. Yang, D. McEachern, S. Przybranowski, E. Fernandez-Salas, B. Wen, D. Sun, S. Wang

MEDI **266.** Glyoxylate shunt as an antibacterial drug target. **S. Bartlett**, A. McVey, A. Crousilles, M. Welch, D.R. Spring

MEDI **267.** Synthesis of monomers with enzymes and chemical reagents for preparing polyester. **K. Kim**, C. Song, K. Jeong, C.S. Cheong

MEDI **268.** Exploit ionic liquids to significantly improve asymmetric reduction of 3,5-bis(trifluoromethyl) acetophenone catalyzed by *T. asperellum* ZJPH0810 cells. **J. Li**, W. Du

MEDI **269.** Microwave-promoted/assisted method for rapid prepararation of biaryl seven-membered lactones. **W. Du**

MEDI **270.** Potent but potentially non-cardiotoxic anthracycline anti-cancer analogs. **J.A. Holdaway**, A.L. Petty, P.L. Barnes, P. Moon, K. Cornell, D.L. Warner

MEDI **271.** Targeting the colchicine binding site in tubulin for cancer treatment: Structural optimization of ABI-231 leads to improved potency and microsomal stability. **Q. Wang**, K. Arnst, D.D. Miller, W. Li

MEDI **272.** Novel, highly selective direct thrombin inhibitors: *In vivo* studies demonstrate efficacy with lower bleeding risk. C. Xu, D. Clemens, S. Dash, K. Lin, M. Reddy, G. Neckermann, S. Yau, E. To, L. Igoudin, S. Chang, S. Keutzer, P. Zalicki, N. Sandoval, S. Sizikov, D. Williams, M. Sivaraja, J. Zhang, T. Shiau, K. Short, **M. Estiarte**, A. Datta, D. Kita

MEDI **273.** Synthesis of a known binder of the GRB2 SH2 domain from naphthaldehyde. **A. Bowlsby**, C. Arpin

MEDI **274.** Novel synthetic strategies to disarm the myeloid cell leukemia-1 oncoprotein. **S.J. Hughes**, B. Drennen, M.E. Lanning, S. Fletcher

MEDI **275.** Improving the *in vitro* and *in vivo* performance of a ^{177}Lu-labeled phosphoramidate-based PSMA inhibitor with an albumin-binding motif. **C.J. Choy**, X. Ling, J.J. Geruntho, S. Beyers, J. Latoche, B. Langton-Webster, C.J. Anderson, C.E. Berkman

MEDI **276.** Synthesis and evaluation of phenyl tetrazole derivatives with amide or urea linkers as BCRP/ABCG2 inhibitors. **N. Gujarati**, L. Zeng, Z. Chen, V.L. Korlipara

MEDI **277.** Two-faced synthetic α-helix mimetics based on heterocyclic cores as dual BCL-2/MDM2 inhibitors. I.L. Conlon, **B. Drennen**, M.E. Lanning, L. Chen, S.J. Hughes, P.T. Wilder, S. Fletcher

MEDI **278.** Kröhnke pyridine synthesis permits facile access to novel Mcl-1 inhibitors. **I.L. Conlon**, D. Van Eker, J. Chauhan, P.T. Wilder, S. Fletcher

MEDI **279.** Dual stimuli-activatable oxidative stress amplifying hybrid anticancer drugs. **J. Noh**, D. Yoo, E. Jung, D. Lee, **J. Lee**

MEDI **280.** Covalent-docking based protocol for the rational design of covalent inhibitors. **X. Wan**

MEDI **281.** Study of the chemical composition, cytotoxic and antitumor activities of *Croton discolor*. **A.D. Ramos Vicente**

MEDI **282.** *Trypanosoma cruzi* sirtuin-2 construction by modeling threading and molecular dynamics. **G.M. Monteiro Ferreira**, G.H. Trossini, F.D. Emery, V.G. Maltarollo

MEDI **283.** DFGmodel: Modeling protein kinases in inactive conformations and its applications in drug discovery. **P. Ung**, A. Schlessinger

MEDI **284.** Virtual screening for potential inhibitors of neuraminidase for influenza treatment. **E.C. Gomez-Suarez**

MEDI **285.** Anthranilic acid derivatives as potential multi-target drugs for metabolic syndrome treatment. **A. Bravo**, H. González Álvarez, M. Loza-Mejía

MEDI **286.** Design and synthesis of N-substituted acridone derivatives as potential antibacterial and antiviral agents. **L.J. Jimenez Sanchez**, D. Juan-Guadarrama, M. Loza-Mejía

MEDI **287.** Developing a chimeric heterobivalent platform as a selective imaging probe for MMP-14. **M. Pun**, R. Rios, C.E. Berkman

MEDI **288.** Structural characterization, homology modelling and virtual screening studies in shikimate kinase from methicillin resistant *Staphylococcus aureus*. **A. Favela**, A. Téllez-Valencia, H. Nájera, J. Cisneros, M. Gómez-Palacio, A. Hernandez Campos, C.I. Avitia-Domínguez

MEDI **289.** Selective inactivation of triosephosphate isomerase from *Trypanosoma brucei*. **A.G. Vazquez-Raygoza**, I. Betancourt, R. Castillo-Bocanegra, C.I. Avitia-Domínguez, E. Sierra, M. Valdez-Solana, A. Téllez-Valencia

MEDI **290.** Design, synthesis, and biological evaluation of novel C3-sustituted β-carboline-based HDAC inhibitors with potent antitumor activities. **Y. Ling**, J. Feng, J. Miao, J. Guo, Y. Peng, Y. Zhang

MEDI **291.** Design and development of reversible inhibitors of lysine specific demethylase 1. **D.P. Mould**, A. McGonagle, M. Geitmann, U. Bremberg, A.M. Jordan, D. Ogilvie

MEDI **292.** Withdrawn.

MEDI **293.** Development of allosteric hydrazide-containing class I histone deacetylase inhibitors for use in acute myeloid leukemia. **J.J. McClure**, C. Zhang, E.B. Inks, Y.K. Peterson, J. Li, C. Chou

MEDI **294.** Withdrawn.

MEDI **295.** Translational feasibility of novel methionyl-tRNA synthetase inhibitors. **M. Bassiri**

MEDI **296.** Identification and development of small molecule inhibitors of the aggregation of amyloid β. **S. Collins**, F. Gielen, L. van Vliet, G. Kaminski, F. Hollfelder, D.R. Spring

MEDI **297.** Drug-target residence time affects *in vivo* drug efficacy through multiple pathways. **K.S. Lee**, J. Yang, K. Wagner, C.J. Ng, J. Niu, A. Dickson, B.D. Hammock

MEDI **298.** Cytotoxicity study of α-hydroxy-β-dicarbonyl bearing synthetic metabolites of poecilosclerid sponge. **S.V. Malhotra**, M.P. Doyle, P. Truong, D. Sharma, A. Nagalingam, W.C. Reinhold, J.R. Alleyn, Y. Yu

MEDI **299.** Second-generation fluorescent ligands for nicotinic acetylcholine receptors. **R.W. Fitch**

MONDAY MORNING

Section A

Moscone Center

3002/3004

Actually it does Work: Success with Allosteric Kinase Ligands & Phosphatase Modulators

L. Lombardo, D. S. Weinstein, *Organizers*

R. Moslin, J. B. Schwarz, *Organizers*, *Presiding*

9:00 MEDI **300.** Discovery of ARQ 092: A potent, selective allosteric inhibitor of AKT1, 2, 3 and AKT1-E17K in clinical development for cancer and rare diseases. **J. Lapierre**, S. Eathiraj, Y. Yu, R.E. Savage, G. Abbadessa, B. Schwartz

9:30 MEDI **301.** Allosteric inhibitors of Interleukin-2-inducible T cell kinase that selectively target its inactive conformation. **A.E. Aulabaugh**

10:00 MEDI **302.** BCR-ABL allosteric inhibitors targeting the myristoyl pocket: Optimization and pharmacological evaluation of substituted N-(4-(trihalomethoxy)phenyl)nicotinamide derivatives towards ABL001. **J. Schoepfer**

10:30 Intermission.

10:40 MEDI **303.** Identifying allostery in signaling enzymes. **W. Peti**

11:10 MEDI **304.** Selective inhibition of a phosphatase to treat neurodegenerative diseases. **A. Bertolotti**

11:40 MEDI **305.** Allosteric inhibition of SHP2 phosphatase. J. Garcia Fortanet, C. Chen, Y. Chen, Z. Chen, Z. Deng, B. Firestone, P. Fekkes, M. Fodor, P. Fortin, C. Fridrich, D. Grunenfelder, S. Ho, Z. Kang, R. Karki, M. Kato, N. Keen, L. Labonte, J. Larrow, F. Lenoir, G. Liu, S. Liu, F. Lombardo, D. Majumdar, M. Meyer, M.G. Palermo, L. Perez, M. Pu, T. Ramsey, W. Sellers, M.D. Shultz, T. Stams, C. Towler, P. Wang, S. Williams, J. Zhang, **M.J. LaMarche**

Section B

Moscone Center

3006/3008

Residence Time: Not Just Affinity for Drug Design

B. Blagg, *Organizer*

P. J. Tonge, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 MEDI **306.** Drug-target residence time model: A 10-year retrospective. **R. Copeland**

9:10 MEDI **307.** Protein dynamics and allostery in kinase activation. **N. Ahn**

9:45 MEDI **308.** Drug target residence time in the early drug discovery phase: HSP90, a model to gain insight into the molecular mechanism of kinetics. **M. Frech**

10:20 MEDI **309.** Determination of *in vivo* enzyme occupancy utilizing inhibitor dissociation kinetics. **M. Lai**, D. Murphy, Y. Ou, D. Euler, K. Wessner, S. Adamski, B. Luo, G. Wesolowski, R. Vogel, H. Glantschnig, L. Lubbers, S. Carroll

10:55 MEDI **310.** Linking target engagement and *in vivo* drug activity: Insights into target vulnerability. **P.J. Tonge**, F. Daryaee, Z. Zhang, K. Gogarty, S.L. Fisher

11:30 Concluding Remarks.

Advances in High-Throughput Screening

Sponsored by CINF, Cosponsored by COMP and MEDI

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

MONDAY AFTERNOON

Section A

Moscone Center

3002/3004

Kinase Inhibitors for Immuno-Inflammatory Diseases

J. Ramanjulu, *Organizer, Presiding*

L. Krim Gavrin, *Presiding*

2:00 MEDI **311.** Discovery of GDC-0853: A potent & selective BTK inhibitor for the treatment of lupus & rheumatoid arthritis. **W.B. Young**

2:30 MEDI **312.** Development of the selective, allosteric RIPK1 kinase inhibitors. M. Najjar, C. Suebsuwong, S. Ray, G. Cuny, **A. Degterev**

3:00 MEDI **313.** Identification of a first-in-class RIP1 kinase inhibitor in phase 2a clinical trials for immuno-inflammatory diseases. **P.A. Harris**

3:30 MEDI **314.** Targeting NF-kB pathways in toll-like receptor and antigen receptor signaling. **H. Wu**

4:00 MEDI **315.** Approaches to TYK2 pseudokinase: A unique mode of allosteric kinase inhibition. **R. Moslin**, S. Wrobleski, Y. Zhang, S. Lin, D. Gardner, J.B. Santella, J.V. Duncia, C. Liu, J. Lin, S. Spergel, M. Mertzman, J.S. Tokarski, H. Sun, M. Chiney, P.A. Elzinga, N. Aranibar, A. Chimalakonda, J. Strnad, A. Zupa-Fernandez, L. Cheng, K. Gillooly, K. Mcintyre, P.H. Carter, L. Lombardo, J. Burke, J.E. Macor, D.S. Weinstein

4:30 MEDI **316.** Design of JAK3 covalent inhibitors for the interrogation of JAK3 signaling in humans. **A. Casimiro-Garcia**, A. Thorarensen, J. Telliez, P. Balbo, M.E. Banker, M.F. Brown, Y. Che, J. Chrencik, J.W. Coe, R. Czerwinski, M.E. Dowty, A.M. Gilbert, M.M. Hayward, M. Hegen, B. Juba, J. Jussif, J. Langille, L. Leung, S. Liang, T. Lin, J.I. Montgomery, S. Soucy, J. Trujillo, R. Unwalla, F.F. Vajdos, F. Vincent, X. Yang

Section B

Moscone Center

3006/3008

Misfolded Proteins in Neurodegenerative Diseases

A. M. Walji, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 MEDI **317.** Targeting intrinsically disordered proteins: Taming alpha-synuclein with small molecules. J. Tao, A. Berthet, D. Agard, **L. McConlogue**

2:10 MEDI **318.** Current status of the development of PET radiotracers for imaging alpha synuclein aggregates in Lewy bodies and Lewy neurites. **R.H. Mach**

2:45 MEDI **319.** HDAC6 inhibitors, autophagy, mitochondrial movement, and disease modification. **A.P. Kozikowski**

3:20 Intermission.

3:35 MEDI **320.** Imaging mutant huntingtin aggregates: Development of potential PET ligand. **C. Dominguez**

4:10 MEDI **321.** Small molecule modulators of ER stress for the treatment of neurodegenerative diseases. **N.D. Cosford**, H. Zou, A. Limpert, J. Zou, A. Dembo, D. Grant, R. Ardecky, A. Pinkerton, G. Magnuson, M. Goldman, J. Rong, D. Sheffler, J. Reed

‡ *Cooperative Cosponsorship*

4:45 MEDI **322.** Discovery of the P7C3 class of neuroprotective compounds. **J. Ready**

5:20 Concluding Remarks.

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Advances in High-Throughput Screening

Sponsored by CINF, Cosponsored by COMP and MEDI

Eminent Scientist Lecture with Dr. Carolyn Bertozzi

Sponsored by SOCED, Cosponsored by MEDI

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

A. W. Stamford, *Organizer*

8:00 - 10:00

111-112, 117, 136, 148, 154, 177, 182, 216, 234, 242, 245, 258, 266, 277, 290. See previous listings.

452, 457, 462, 473. See subsequent listings.

TUESDAY MORNING

Section A

Moscone Center

3002/3004

MEDI Awards Symposium

A. W. Stamford, *Organizer*

W. B. Young, *Presiding*

9:00 MEDI **323.** Withdrawn.

9:45 MEDI **324. Award Address** (E. B. Hershberg Award for Important Discoveries in Medicinally Active Substances sponsored by Merck Research Laboratories). Present and future of antisense technology. **S. Crooke**

10:30 MEDI **325. Award Address** (ACS Award for Creative Invention sponsored by ACS Corporation Associates). CPP-115: A novel GABA aminotransferase inactivator and potential new treatment for epilepsy, addiction, and hepatocellular carcinoma. **R.B. Silverman**

11:15 MEDI **326.** Bristol-Myers Squibb Smissman award lecture: Receptor structures enable drug discovery. **K.A. Jacobson**

Section B

Moscone Center

3006/3008

Antibiotic Drug Discovery: The Next Frontier

E. D. Brown, C. L. Freel Meyers, *Organizers*, *Presiding*

8:30 MEDI **327.** Targeting bacterial bioenergetics and central metabolism: Challenges and opportunities. **K. Pethe**

9:10 MEDI **328.** Targeting bacterial nutrient biosynthesis with natural products. **E.D. Brown**

9:50 MEDI **329.** Antibacterial agents that target adenylating enzymes in *Mycobacterium tuberculosis*. **C.C. Aldrich**

10:30 MEDI **330.** Targeting a branch point in bacterial metabolism through inhibition of DXP synthase. **C.L. Freel Meyers**

11:10 MEDI **331.** Co-therapy strategy to enhance target vulnerability in *Mycobacterium tuberculosis*. **N.S. Sampson**

11:50 MEDI **332.** Discovery of ETX2514, a novel, rationally designed inhibitor of class A, C and D β-lactamases, for the treatment of Gram-negative infections. **T.F. Durand-Reville**

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡

TUESDAY AFTERNOON

Section A

Moscone Center

3002/3004

Drug Discovery for ALS: Putting the Ice Bucket to Work

L. Bruijn, G. M. Dubowchik, *Organizers*, *Presiding*

2:00 MEDI **333.** Challenges and opportunities for drug discovery in ALS. **L.I. Bruijn**

2:40 MEDI **334.** Identification and preclinical pharmacology of antisense oligonucleotides targeted to human SOD1 for the treatment of ALS. **E.E. Swayze**

3:20 MEDI **335.** Design and study of small molecules targeting r(G4C2) repeats in ALS and FTD. **M.D. Disney**

4:00 Intermission.

4:15 MEDI **336.** Dual leucine zipper kinase inhibitors for the treatment of neurodegenerative diseases. **M. Siu**

4:55 MEDI **337.** Development of small-molecule autophagy inducers that mitigate neurodegeneration in models of ALS and other disorders. **S. Finkbeiner**

Section B

Moscone Center

3006/3008

General Orals

A. W. Stamford, *Organizer*

A. Ali, *Presiding*

1:30 MEDI **338.** γ-Functionalized hydrocarbon stapled peptides for inhibiting mutant estrogen receptor/coactivator interaction. **T. Speltz**, C.G. Mayne, S. Fanning, E. Tajkhorshid, G. Greene, T.W. Moore

1:55 MEDI **339.** Discovery of BMS-986104: Moving from direct-acting, full agonists to pro-drug, partial agonists in the identification of a differentiated S1P1 modulator with an improved safety profile. **A.J. Dyckman**, M. Dhar, D. Marcoux, H. Xiao, Z. Xiao, J.L. Gilmore, L. Li, A. Mathur, J. Xie, X. Yang, T.L. Taylor, R. Thomas, K. Mcintyre, L. Lehman-McKeeman, H. Shi, P. Levesque, P. Balimane, H. Sun, A.M. Marino, Z. Yang, D. Shen, M. Cvijic, B.M. Warrack, G. Cornelius, C.J. D'Arienzo, L. Salter-Cid, J.C. Barrish, P.H. Carter

2:20 MEDI **340.** Phenotypic screening identifies a small molecule anti-secretagogue of PCSK9 that acts via a novel mechanism of action. D. Petersen, J. Hawkins, W. Ruangsiriluk, K. Stevens, B. Maguire, T.N. O'Connell, B.N. Rocke, M. Boehm, R.B. Ruggeri, T. Rolph, D. Hepworth, P. Loria, **P.A. Carpino**

2:45 MEDI **341.** Discovery of chemical biology probes inhibiting activation of SGK3 kinase in cancer cells. **M. Lindvall**, G.A. Nishiguchi, C. Bellamacina, W. Shu, L. Tian, E.J. Martin, S. Ma, E. Fang, T. Zavorotinskaya, E. Park, D. Duhl, A.C. Rico, V. Tamez, L. Doyle, M. Doyle

3:10 MEDI **342.** Unveiling the truth about PAK1 with medicinal chemistry. **J. Rudolph**, L.J. Murray, C.O. Ndubaku, T. O'Brien, E. Blackwood, W. Wang, I. Aliagas, L.J. Gazzard, J.J. Crawford, J. Drobnick, W. Lee, X. Zhao, D. Favor, P. Dong, H. Zhang, C.E. Heise, A. Oh, C. Ong, H. La, P. Chakravarty, C. Chan, D. Jakubiak, J. Epler, S. Ramaswamy, R. Vega, G. Cain, D. Diaz, Y. Zhong

3:35 MEDI **343.** Discovery of the potent and selective, broad spectrum fungal CYP51 inhibitor VT-1598. **C.M. Yates**, E.P. Garvey, R.J. Schotzinger, S.R. Shaver, W.J. Hoekstra

4:00 MEDI **344.** Discovery of the brain penetrant Phosphodiesterase 1 (PDE1) inhibitor Lu AF64386. **J. Kehler**, A.I. Parachikova, H. Lindgren, L.K. Rasmussen, M. Langgard, C.T. Christoffersen, C. Bundgaard, K. Juhl, L. Skibsbye, J. Agner, J. Nielsen

4:25 MEDI **345.** Impact of P-gp susceptibility on brain penetration for a series of potent, selective, and orally bioavailable TrkA inhibitors. **M.E. Fraley**

4:50 MEDI **346.** Discovery of ruzasvir (MK-8408), a 2nd generation HCV NS5A inhibitor. **W. Yu**, L. Tong, L. Chen, O. Selytin, M.P. Dwyer, A.G. Nair, R. Mazzola, J. Kim, D. Sha, J. Yin, R. Ruck, I.W. Davies, B. Hu, B. Zhong, J. Hao, T. Ji, S. Zan, R. Liu, S. Agrawal, E. Xia, S. Curry, P. Mcmonagle, K. Bystol, F. Lahser, D. Carr, L. Rokosz, P. Ingravallo, S. Chen, K. Feng, M. Cartwright, E. Asante-Appiah, J.A. Kozlowski

Entrepreneurship in Biotechnology, Advanced Materials, Drug Discovery & Information Systems

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ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

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Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

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WEDNESDAY MORNING

Section A

Moscone Center

Gateway Ballroom 103/104

First Time Disclosures

J. B. Schwarz, *Organizer, Presiding*

8:00 MEDI **347.** Discovery of highly efficacious potentiators for the treatment of cystic fibrosis. **S. Van der Plas**, H. Kelgtermans, T. De Munck, S. Martina, L. Tomaskovic, T. Christophe, M. Jans, E. Van der Aar, M. Borgonovi, L. Nelles, M. Gees, P. Stouten, J. Van Der Schueren, O. Mammoliti, M. Andrews, K. Conrath

8:30 MEDI **348.** Discovery of ABBV/GLPG-2222: A potent, efficacious CFTR corrector for the treatment of cystic fibrosis. **X. Wang**

9:00 MEDI **349.** Discovery of clinical candidate BMS-986158, an oral BET inhibitor for the treatment of cancer. **A.V. Gavai**, D. Norris, G.V. De Lucca, D. Tortolani, D.P. O'Malley, Y. Zhao, C.A. Quesnelle, W. Han, P. Gill, W. Vaccaro, T. Huynh, V. Ahuja, D. Dodd, C. Mussari, L.S. Harikrishnan, M. Kamau, J.S. Tokarski, R. Rampulla, D. Wu, J. Li, H. Zhang, P. Li, D.Z. Sun, H. Yip, C. Wang, Y. Zhang, A. Mathur, H. Zhang, C. Huang, Z. Yang, A. Ranasinghe, C.J. D'Arienzo, C. Tye, C. Su, G. Everlof, L. Zhang, N. Raghavan, K. Menard, M. Wen, J.T. Hunt, M. Poss, G. Vite, R. Westhouse, F. Lee

9:30 MEDI **350.** Discovery of a novel class of potent, selective, and orally bioavailable histone methyltransferase Enhancer of Zeste Homolog 2 (EZH2) inhibitors and the identification of development candidate PF-06821497. **P. Kung**, S. Bergqvist, P. Bingham, J.F. Braganza, A. Broun, M.R. Collins, W. Diehl, Y. Deng, D. Dinh, C. Fan, V.R. Fantin, H.J. Gukasyan, W. Hu, B. Huang, R. Kania, W. Liu, S. Kephart, M. Kraus, C. Krivacic, R.A. Kumpf, G. Li, K. Maegley, I.J. McAlpine, L. Nguyen, S. Ninkovic, M.A. Ornelas, D. Richter, E. Rui, M. Ryskin, S.A. Scales, J. Spangler, A. Stewart, S.C. Sutton, J. Tatlock, C. Tsao, D. Verhelle, F. Wang, H. Wang, P. Wells, M. Wythes, S. Yamazaki, B. Yip, X. Yu, L. Zehnder, W. Zhang, P. Zhu, J. Zhu, R.A. Rollins, S. Sharma, M.P. Edwards

10:00 MEDI **351.** Discovery and development of BLU-554: A potent, highly selective covalent inhibitor of Fibroblast Growth Factor Receptor 4 (FGFR4) in development for the targeted treatment of advanced Hepatocellular Carcinoma (HCC) patients with amplified and overexpressed FGF19. **C.V. Miduturu**, M. Hagel, M. Sheets, N. Rubin, W. Weng, N. Bifulco, L.V. Dipietro, J. Kim, N. Brooijmans, B.L. Hodous, N. Stransky, K. Hoeflich, V.J. Kadambi, N. Kohl, C. Lengauer, T. Guzi

10:30 MEDI **352.** Discovery of PRN1371: A highly selective, irreversible inhibitor of FGFR1-4 in clinical development for the treatment of solid tumors. **K.A. Brameld**

11:00 MEDI **353.** FGF401: A reversible-covalent inhibitor of FGFR4 for the treatment of hepatocellular carcinoma. **R.A. Fairhurst**, T. Knoepfel, P. Furet, N. Buschmann, C. Leblanc, R. Mah, M. Kiffe, D. Graus-Porta, A. Weiss, J. Kinyamu-Akunda, M. Wartmann, J. Trappe, T. Gabriel, F. Hofmann, W. Sellers

11:30 MEDI **354.** Interdiction at a protein-protein interface: Structure-based design of the Mcl-1 inhibitor AMG 176. **S.P. Brown**

Section B

Moscone Center

3006/3008

Targeting Epigenetic Writers & Erasers

J. Jin, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 MEDI **355.** Probing the epigenome for therapeutic targets. **C.H. Arrowsmith**

9:05 MEDI **356.** Tazemetostat, a first-in-class inhibitor of EZH2: From bench to bedside to bench. **R. Copeland**

9:35 MEDI **357.** Sirtuin inhibitors as promising anticancer agents. **H. Lin**

10:05 Intermission.

10:20 MEDI **358.** Targeting histone lysine methylation regulatory pathways in cancer. **P. Trojer**

10:50 MEDI **359.** Exploring novel models of interaction to inhibit protein methyltransferases. **M. Luo**

11:20 MEDI **360.** Chemical probes targeting the protein arginine deiminases. **P.R. Thompson**

11:50 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Moscone Center

Gateway Ballroom 103/104

First Time Disclosures

J. B. Schwarz, *Organizer, Presiding*

1:30 MEDI **361.** Discovery of clinical candidate PF-06648671: A potent, highly brain penetrant gamma secretase modulator for the treatment of Alzheimer's disease. **M. Pettersson**, C. am Ende, T.W. Butler, P.H. Dorff, I.V. Efremov, E. Evrard, S.A. Eisenbeis, C.J. Helal, M.E. Green, J.M. Humphrey, G.W. Kauffman, P.B. Mullins, C.J. O'Donnell, D.A. Rankic, A.F. Stepan, C.M. Stiff, N. Patel, C. Subramanyam, T.P. Tran, E.X. Yang, L. Xie, K.R. Bales, E. Hajos-Korcsok, B.A. Pettersen, L.R. Pustilnik, S.J. Steyn, K.M. Wood, R. Qiu, P.R. Verhoest

2:00 MEDI **362.** Discovery of a small molecule αvβ6 inhibitor for idiopathic pulmonary fibrosis. **S.J. MacDonald**, J. Pritchard, N. Anderson

2:30 MEDI **363.** Identification of AZD9567, an anti-inflammatory glucocorticoid receptor modulator with improved side effect profile. **L. Ripa**, M. Dearman, G. Edenro, K. Edman, R. Hendrickx, M. Lepistö, L. Öberg

3:00 MEDI **364.** Discovery and early clinical profile of a non-catchol dopamine 1 receptor agonist. **D.L. Gray**, R. Kozak, S. Mente, J.E. Davoren, D. Nason, S. ONeil, I.V. Efremov, A. Harris, R. O'Connor, M. Salafia

3:30 MEDI **365.** Discovery and development of BLU-285: A potent, highly selective inhibitor of KIT and PDGFRα activation loop mutants. **B.L. Hodous**, E. Evans, A. Gardino, A. Davis, J. Zhu, D.P. Wilson, K. Wilson, L.V. Dipietro, J. Kim, N. Brooijmans, V.J. Kadambi, A. Shutes, Y. Zhang, N. Kohl, C. Lengauer, T. Guzi

4:00 MEDI **366.** NVP-LXS196, a novel PKC inhibitor for the treatment of uveal melanoma. **M. Visser**, J.P. Papillon, J. Fan, M. Luzzio, W. Michael, R. Wang, A. Zhang, C. Straub, S. Mathieu, M. Kato, M.G. Palermo, C. Chen, M.J. LaMarche, T.M. Ramsey, A. Vattay, R. Guo, V. Cooke, A. Bric, F. Chung, G. Liang, M. Romanowski, A. Wylie

4:30 MEDI **367.** Discovery of selonsertib (GS-4997): A first in class, selective inhibitor of apoptosis signal-regulating kinase 1. **G.T. Notte**, B. Corkey, E. Lansdon, D. Breckenridge, O.L. Saunders, M. Graupe, B. Murray, C. Venkataramani, J. Guerrero, J. Farand, J.A. Zablocki, K. Babaoglu, J. Liles, G. Budas, S. Wise, K. Koch, L. Castonguay, M.C. Desai

5:00 MEDI **368.** Discovery of a selective inhibitor of indoleamine-2,3-dioxygenase for use in the therapy of cancer. **A. Balog**

Section B

Moscone Center

3006/3008

General Orals

A. W. Stamford, *Organizer*

J. Ramanjulu, *Presiding*

1:30 MEDI **369.** Teaching old drugs new tricks: Reprogramming ethionamide's bioactivation to fight multidrug resistant *Mycobacterium tuberculosis*. **N. Willand**, M. Gitzinger, B. Deprez, A. Baulard

1:50 MEDI **370.** Preclinical development and characterization of MYC inhibitors. **N. Jacob**, P. Miranda, P. Serrano Navarro, J. Hart, P.K. Vogt, K.D. Janda

2:10 MEDI **371.** Discovery of PF-06748962: A potent and selective lactam-based EP3 antagonist. **K. Futatsugi**

2:30 MEDI **372.** Novel pyrrolomycins as potent antibacterial agents against *ESKAPE* pathogens and biofilms. **R. Li**, Z. Yang, J. Ahn, Y. Liu, Y. Chhonker, D. Murry, H.A. Zhong, K. Bayles

2:50 MEDI **373.** Development and application of an NMR-based activity and inhibition assay for mycobacterial isocitrate lyase. **R.P. Bhusal**, K. Patel, B. Kwai, G. Bashiri, J. Reynisson, J. Sperry, I.K. Leung

3:10 MEDI **374.** LEGO®-inspired drug design: Discovery of novel fungal Plasma membrane H^+-ATPase (Pma1) inhibitors from small molecule libraries: An introduction of HFSA-SBS_DOS-RD strategy in drug discovery. **T. Tung**, T. Dao, M.B. Palmgren, A.T. Fuglsang, S.B. Christensen, **J. Nielsen**

3:30 MEDI **375.** Reducing cycle time in medicinal chemistry drug discovery. **J.S. Wai**, T. Wang

3:50 MEDI **376.** Enzymatic tandem carboxylation-amidation as a bioactivity-potentiating strategy in the production of natural and unnatural thiolactomycin antibiotics. **J. Li**, X. Tang, S. Mckinnie, T. Awakawa, B.S. Moore

4:10 MEDI **377.** Structure-based design of highly potent small-molecule inhibitors of DCN1-UBC12 protein-protein interaction. **H. Zhou**, J. Lu, L. Liu, D. Bernard, J. Stuckey, Y. Sun, S. Wang

4:30 MEDI **378.** CDK8 inhibitors with long residence time emerging from a retro-design approach: New opportunities for cancer treatment. J.C. Benningshof, B. Aerts, **G. Müller**, J. Veerman, E. Damen, M. Kubbutat, J. Ehlert, H. Holger, F. Totzke

4:50 MEDI **379.** Structure-based design, synthesis, biological evaluation, and x-ray crystallographic analysis of novel, highly potent HIV-1 protease inhibitors to address multi-drug resistant HIV. A.K. Ghosh, **H.L. Osswald**, J. Agniswamy, Y. Wang, I. Weber, M. Amano, H. Mitsuya

WEDNESDAY EVENING

Section A

Moscone Center

West Hall

General Posters

A. W. Stamford, *Organizer*

7:00 - 9:00

MEDI **380.** Inhibition of Aβ-40 and Aβ-42 aggregation by piceatannol and cis-piceatannol. **J.M. Chapman**, M. Moss, Y. Wang

MEDI **381.** Photoelectrocatalytic inhibition of Alzheimer's β-amyloid aggregation in vitro by hole-derived radicals. **K. Kim**, B. Lee, Y. Chung, W. Choi

MEDI **382.** Synthesis of Yakuchinone-derived compounds that inhibit β-amyloid aggregation. **L. Chen**, C. Yen, H. Tseng, Y. Huang, Y. Lu, W. Hou, K. Hsu, I. Pan, K. Huang, W. Huang

MEDI **383.** Photoexcited ruthenium complex for highly sensitive inhibition of β-amyloidogenesis. **G. Son**, C. Park, B. Lee, Y. Chung

MEDI **384.** New hydroxyquinoline-based derivatives as potent modulators of amyloid-b aggregations. **M. Hu**

MEDI **385.** Potential multimechanistic therapeutic effects of dihydropyridine calcium channel blockers: Mechanistic study of effects on amyloid-beta aggregation associated with Alzheimer's disease. **J.M. Chapman**, M. Moss, J. Tseng

MEDI **386.** Withdrawn.

MEDI **387.** Development of MBRI-001, a deuterium-substituted plinabulin, as a potent anti-microtubule agent for anticancer. Z. Ding, H. Cheng, S. Wang, Y. Hou, J. Zhao, H. Guan, **W. Li**

MEDI **388.** β-Sheet propensity of competitive peptide inhibitor's residue is crucial in binding to proteases: PACE4 inhibitors as a case study. **V. Dianati**, A. Shamloo, A. Kwiatkowska, R. Desjardins, A. Soldera, R. Day, Y. Dory

MEDI **389.** Hepsin-targeted ligands for prostate cancer imaging and therapy. **Y. Byun**, S. Son, H. Kwon

MEDI **390.** X-ray crystallographic structures of teixobactin analogues. **H. Yang**, D.R. Du Bois, J.W. Ziller, J.S. Nowick

MEDI **391.** Withdrawn.

MEDI **392.** Long wavelength, orthogonal release of internalized anti-inflammatory compounds from cellular vehicles. **R.M. Hughes**, C. Marvin, Z. Rodgers, S. Ding, N. Oien, W.J. Smith, D.S. Lawrence

MEDI **393.** Amino acid and peptide conjugates are potential drug candidates. **S.S. Panda**

MEDI **394.** Withdrawn.

MEDI **395.** Directed immune responses via covalently linked TLR agonist combinations for a Q-fever vaccine. **T.J. Albin**, J. Tom, S. Manna, A. Gilkes, A. Jain, M. Supnet, H. Davies, A. Nalca, A. Burkhardt, P. Felgner, A.P. Esser-Kahn

MEDI **396.** Development of antidotes against nerve agent inhibited acetylcholinesterase – the transformation of an inhibitor into a reactivator. **C. Lindgren**, N. Forsgren, C. Akfur, L. Berg, D. Andersson, M. Hillgren, W. Qian, F. Worek, F. Ekström, A. Linusson

MEDI **397.** Generating site-specific antibody-drug conjugates with high drug to antibody ratios using a tandem Knoevenagel dondensation-Michael addition. **R. Kudirka**, R. Barfield, J. McFarland, P. Drake, A. Carlson, S. Banas, W. Zmolek, A. Garofalo, D. Rabuka

MEDI **398.** Synthesis of truncated tirandamycin A-D derivatives as new antihelminthic agents. **T. Jimenez**, M. Grotli, C. Wallentin

MEDI **399.** Beyond IC50 and simple PK models – considerations for discovery chemists. **R. Fraczkiewicz**, M.B. Bolger, W. Woltosz

MEDI **400.** Synthesis and evaluation of antitubercular agents 2-aminothiophenes and benzo-1,2-selenazol-3(2H)-ones targeting Pks13 and Ag85C respectively. **S. Thanna**, S.E. Knudson, C.M. Goins, F. Salem, S. Kapil, A. Grzegorzewicz, M. Jackson, D.R. Ronning, R.A. Slayden, S.J. Sucheck

‡ *Cooperative Cosponsorship*

MEDI **401.** Novel pyrimidine compounds as potent JAK inhibitors. **Y. Chen**, H. Li, R. Yen, T. Heckrodt, D. McMutrie, N. Lin, R. Singh, V. Taylor, M. Chan, E. Masuda, G. Park, D. Lau, D. Payan

MEDI **402.** Synthesis and evaluation polythiophene containing rhodamine dyes for biological and photochemical applications. **M.K. Linder**, J.N. Nasca, K.S. Gast, G. Sawada, D. Watson, M.R. Detty

MEDI **403.** Synthesis of β-configured clickable [^{18}F]FDGs as novel ^{18}F-fluoroglycosylation tools for PET *in vivo* imaging. **M. Elgland**, P. Nordeman, T. Fyrner, P. Konradsson, G. Antoni, P. Nilsson

MEDI **404.** Small-molecule anti-virulence agents for the prevention of dental biofilms. **B. Nijampatnam**, H. Wu, S.E. Velu

MEDI **405.** Discovery of novel pyrrolomycins as potential anticancer agents. **Y. Liu**, T. McGuire, Z. Yang, D. Coulter, Y. Chhonker, D. Murry, J. Sharp, H.A. Zhong, **R. Li**

MEDI **406.** Design and synthesis of small molecule inhibitors bearing 1,2,3-triazole/sulfonate pharmacophore from natural precursors for the treatment of bacterial infections. **B. Aneja**, S. Alam, M. Azam, A. Perwez, R. Haque, M. Rizvi, R. Maguire, K. Kavanagh, U. Yadava, C. Daniliuc, A. Azam, A. Mohammad

MEDI **407.** New N-substituted indazole-5-carboxamides as subnanomolar, selective monoamine oxidase B and dually active MAO-A/B inhibitors with BBB and GI permeability. **M. Gastreich**, C. Detering, L. Antonov, S. Hristova, H. Stammler, N.T. Tzvetkov

MEDI **408.** Withdrawn.

MEDI **409.** Glycosylated porphyrins for use in PET and PDT: Synthesis and characterization. **K. Arja**, M. Elgland, P. Nilsson

MEDI **410.** Selective nicotinic acetylcholine receptor activities from the areca nut. **N. Horenstein**, C. Stokes, R. Papke

MEDI **411.** Withdrawn.

MEDI **412.** Differentiating antiproliferative and chemopreventive modes of activity for electron-deficient aryl isothiocyanates against human MCF-7 cells. **J.R. Mays**

MEDI **413.** Application of the boronic acid as an isostere of the phenolic hydroxyl group in optimization of Selective Estrogen Receptor Downregulators (SERDs). **J. Liu**, S. Zheng, S. Guo, Q. Zhong, M. Bratton, T.E. Wiese, G. Wang

MEDI **414.** Withdrawn.

MEDI **415.** Substituted acylsulfonamides as surrogates of a terminal carboxylic acid: More effective small-molecule blockade of the Mcl-1 oncoprotein. **M.E. Lanning**, S. Fletcher

MEDI **416.** Novel class of substituted phenoxyacetamide derivatives as serotonin reuptake inhibitors and serotonin autoreceptor antagonists for repetitive behavior modulation in autism spectrum disorder. V.M. Gancarczyk, J. Dhuguru, A. Khalil, **O.M. Ghoneim**

MEDI **417.** Polymersomes for targeting and eradicating intracellular parasites. **L. Rizzello**, J. Robertson, P. M. Elks, T. McHugh, S. A. Renshaw, G. Battaglia

MEDI **418.** Two-in-one approach to modulate repetitive behaviors in autism spectrum disorder: N-arylpieprazines as key motifs towards developing bi-functional serotonergic ligands. **O.M. Ghoneim**

MEDI **419.** Zinc(II)-dipicolylamine coordination complexes are strongly active against cutaneous leishmaniasis. **M. Betancourt**, D. Rice, P. Vacchina, B. Norris-Mullins, M.A. Morales, B.D. Smith

MEDI **420.** Peptide-based nanosponges. **S.H. Bossmann**, H. Wang, A.S. Yapa, S.O. Wendel, N. Kariyawasam, T.B. Shrestha, M. Pyle, P.E. Smith, D.L. Troyer

MEDI **421.** Heterocyclic mimetics of crinine alkaloids – Novel scaffolds against drug-resistant cancer cells. **L.V. Frolova**

MEDI **422.** Characterization of histone lysine methyltransferase and discovery of NSD2 inhibitors. **J. Kwiatkowski**, A. Hung, Y. Tan, N. Ahmad, G. Lin, A. Ngo, Y. Li, H. Ng, J. Wee, X. Koh-Stenta, P.Z. Kwek, E.H. Ong, J.K. Joy, A. Poulsen, C. Kang, J. Hill, T.H. Keller

MEDI **423.** Computational rationalisation of ligand specific T-cell activation by the lipid presenting proteins CD1b and CD1c: Different means to the same end? **C. Cave-Ayland**, A. Chancellor, I. Tews, S. Mansour, C. Skylaris, J.W. Essex

MEDI **424.** Pharmacophore construction of Cyclooxygenase-2 (COX-2) selective inhibitors based on QSAR models. R.A. Gomes, G.L. Luiz Genesi, V.G. Maltarollo, **G.H. Trossini**

MEDI **425.** Perturbing dissimilar biomolecular targets from natural product scaffolds and focused chemical decoration. **J. Nielsen**, **T. Tung**, T. Holm Jakobsen, T. Dao, A.T. Fuglsang, M. Givskov, S.B. Christensen

MEDI **426.** Design of novel GPCR family-targeted scaffolds: Synthetic and cheminformatic exploration of novel medicinal chemistry space. **J.C. Benningshof**, G. Müller, T. Berkenbosch, D. Stumpfe, J. Bajorath

MEDI **427.** Synthesis and biological evaluation of C24 20*S*(OH)D3 analogs as anti-inflammatory agents. **Z. Lin**, S. Marepally, E. Goh, C.Y. Cheng, A.E. Postlethwaite, Z. Janjetovic, T. Kim, A.J. Slominski, R.C. Tuckey, N. Rochel, D.D. Miller, W. Li

MEDI **428.** Multi-omic approach to unraveling the microbial ecology of *Euphorbia* plant latex. M. Gunawardana, E. Hyde, S. Rivera, S. Webster, A. Castonguay, M. Anderson, S. Lahmeyer, B. Dorsey, T. La Val, D. VanderVelde, P. Webster, R. Knight, **M.M. Baum**

MEDI **429.** Discovery of novel indolinone derivatives as potent MELK inhibitors. **R. Edupuganti**, J.M. Taliaferro, Q. Wang, X. Xie, E.J. Cho, V. Sharma, P. Ren, C. Bartholomeusz, E.V. Anslyn, K.N. Dalby

MEDI **430.** Sphingosine analogues as inhibitors of Sphingosine Kinase (SK1). A. Cardona, M. Escudero-Casao, M. Corro, J. Hernandez, Y. Diaz, I. Matheu, S. Garcia-Vallve, M. Mulero, G. Pujadas, **S. Castillon**

MEDI **431.** Biological screening of *Moringa oleifera* for cytotocixity and antitumor activities. **E.P. Rodriguez**, C.A. Ospina

MEDI **432.** Design of a nucleic acid aptamer to achieve localization of a ROS-activated anti-cancer agent. **K.G. Earnest**, E.J. Merino

MEDI **433.** Exploring the binding site of GPR119 receptor inverse agonists. **E. Kotsikorou**, **S. Kowalski**

MEDI **434.** Methicillin-resistant *Staphylococcus aureus* becomes vulnerable to β-lactam antibiotics when in combination with branched polyethylenimine. **M. Foxley**, M. Xiao, S. Wright, S. Strange, A. Lam, K. Grogan, C.V. Rice

MEDI **435.** Old and new privileged scaffolds for medicinal chemistry. **P. Schneider**, G. Schneider

MEDI **436.** Vienna LiverTox Workspace: Towards predicting liver toxicity. **F. Montanari**, E. Kotsampasakou, B. Knasmüller, M. Pinto, M. Grandits, L. Richter, G.F. Ecker

MEDI **437.** Pyrrole-based antitubulin agents at the colchicine site: SAR of C-5 analogues in explicitly solvated models. **A.J. Obaidullah**, C.C. Rohena, J.A. Sikorski, S. Mooberry, J.T. Gupton, G.E. Kellogg

MEDI **438.** Design, synthesis, and biological evaluation of small molecule Giα2-androgen inhibitors in prostate cancer therapy. **S. Tapadar**, S. Caggia, S. Khan, A.K. Oyelere

MEDI **439.** Synthesis of GRB2 SH2 domain inhibitors: Analogues of sclerotiorin. **J.J. Gladfelder**, C. Arpin

MEDI **440.** Phytoestrogens: New ligands targeting the estrogen receptor domains. **V.J. Thakor**, M. Noolvi

MEDI **441.** Structure-based design of macrocyclic tetrapeptides intended to modulate the opioid receptors. **M.J. Ferracane**, J.V. Aldrich

MEDI **442.** MOEsaic: Making SAR analysis easier through the use of matched molecular pairs and R-group profiling. **A. Ajamian**

MEDI **443.** In search of AKT inhibitors as anticancer agents, an in silico approach. **P.J. Trejo**, A. Hernandez Campos, A. Romo-Mancillas, J.L. Medina-Franco, R. Castillo-Bocanegra

MEDI **444.** Design, synthesis and biological evaluation of Liver X Receptor (LXR) ligands. **R. Komati**, K.M. Lamark, K.A. Payne, M. Ndukwe, D. Spadoni, J. Sridhar, K. Riley

MEDI **445.** Amido phthalimides as CDKs and VEGF inhibitors. **R. Komati**, V.C. Miles, M. Ismail, F. Joseph, H. McFerrin, J. Sridhar

MEDI **446.** Withdrawn.

MEDI **447.** Discovery of Lu AF64196 a highly ligand efficient, brain penetrant and selective PDE1 inhibitor. **L.K. Rasmussen**, M. Langgard, C.T. Christoffersen, J. Nielsen, C. Bundgaard, J. Kehler

MEDI **448.** Repurposing for G-protein couple receptors by structure-based discovery: Transformation of adenosine derivatives into $5HT_{2B}$/$5HT_{2C}$ serotonin receptor antagonists. **D. Tosh**, A. Ciancetta, E.P. Warnick, S. Crane, Z. Gao, K.A. Jacobson

MEDI **449.** Discovery of highly selective Itk inhibitors with *in vivo* IL-2 inhibition. **S. Takai**, H. Takeda, A. Watanabe, K. Tsuboi, R. Suzuki, A. Hiramatsu, Y. Iyoda, T. Inukai, A. Kinoshita, H. Kohno, B. Liu, R. Shetty, K. Moriarty, M. Kurono, S. Umemura, H. Egashira, J. Zou, Z. Konteatis, R. Omi, H. Namboodiri, W. Sawada, M. Murata, T. Koike, R. Komaki-Nishikawa, N. Yada, T. Yoshizawa, J. McCool, M. Bukhtiyarova, M. Kelly, J. Takeuchi

MEDI **450.** Decoupling proton motive force to overcome antibacterial resistance. **J. Buonomo**, C.C. Aldrich

MEDI **451.** Adverse drug reactions triggered by the common HLA-B*57:01 variant: Virtual screening of DrugBank. **G. Van Den Driessche**, D. Fourches

MEDI **452.** Optimization of 4(1*H*)-quinolone antimalarials for oral bioavailability and in vivo efficacy. **C. Lichorowic**, J.R. Maignan, R. Neelarapu, A. Monastyrski, J.V. Giarrusso, T. Mutka, L. Blake, D. Casandra, A. LaCrue, D. Kyle, R. Manetsch

MEDI **453.** Design of inhibitors for the human papillomavirus E6 protein. **D.P. Petrov**, V.J. Davisson, E. Androphy, A. Rietz

MEDI **454.** Scaffold replacement and 3D ligand optimization applied to the discovery of tyrosine kinase inhibitors. **A. Deschenes**

MEDI **455.** Discovery of the first low-molecular-weight *Mycobacterium tuberculosis* MabA (FabG1) inhibitors using a fragment-based approach. C. Pintiala, M. Moune, K. Bourbiaux, R. Frita, K. Djaout, C. Piveteau, B. Deprez, A. Baulard, N. Willand, **M. Flipo**

MEDI **456.** Structure-based, in molecular design and synthesis of inhibitors of protein kinase family of receptors of epidermal growth factor. **A.S. Bunev**, E.V. Sukhonosova, G. Lisnik, N. Yabbarov, G. Ostapenko

MEDI **457.** *In vivo* structure-efficacy studies of regioisomeric artemolane-like endoperoxides. **B.R. Blank**, J. Gut, P.J. Rosenthal, A.R. Renslo

MEDI **458.** Optimization of peptide substrates for conjugate modification of macromolecular mediated RNAi delivery. **J.C. Carlson**, J. Benson, A.V. Blokhin, D. Rozema, A. Sokoloff

MEDI **459.** Impact of activation of GPR68 by metal cations on high throughput screening. **C. Wang**, S. Lin, L.D. Fader, A. Granger

MEDI **460.** Synthesis of 1,2,4-substituted imidazoles for a fragment-based drug discovery library. **T. Lafferty**, J. Patrone

MEDI **461.** Identification and optimization of 5-aryl benzimidazolones as AMPA receptor negative modulators selective for TARP-γ8. **S. Ravula**, **M. Ameriks**, **B.M. Savall**, **J.M. Ziff**, **B.T. Shireman**, **M.J. Seierstad**, **N. Wu**, **B. Lord**, **M. Maher**, **N.I. Carruthers**, **T.W. Lovenberg**

MEDI **462.** Design and synthesis of L-neplanocin analogues as antiviral agents. **Q. Chen**, C. Liu, S. Schneller, **A. Davidson**, **M. Stout**

MEDI **463.** Targeted isolation and simplified structure elucidation of new analogues of dolastatin 10 from marine cyanobacteria using MS/MS molecular networking. **B. Naman**, J. Almaliti, L. Keller, A. Remmel, E. Glukhov, P.C. Dorrestein, W.H. Gerwick

MEDI **464.** MELK as a valid cancer therapeutic target? From virtual screening to highly selective in vivo tool compounds. **S. Mathieu**, B. Toure, J. Giraldes, T. Smith, E. Sprague, Y. Yang, Z. Chen, Y. Mishina, Y. Feng, Y. Yan-Neale, D. Chen, M. Meyer, C. Straub, D. Sage, K. Wright, X. Chen, S. Kim, E.J. Martin, K. Hurov

MEDI **465.** P(NIPAM) microgel embedding p(AAm) hydrogel interpenetrating polymer networks for controlled drug delivery vehicles. **N. Sahiner**, A. Yasar, F. Onder, M. Ay

MEDI **466.** Evaluation of antimicrobial properties of *Combretum laxum* extracts. **J.G. Escobar**, **I. Maldonado**, **A.K. Addo-Mensah**

MEDI **467.** Development of a new class of fluorophores and their applications as biological imaging agents and chemical sensors. **J.R. Zimmerman**

MEDI **468.** Inhibition of pilocarpine-induced fluid secretion by ethylatropine bromide. **T. Ganesh**, A. Rojas, A. Walker, R. Dingledine

MEDI **469.** Structure-Based Drug Design (SBDD) of allosteric inhibitors for HSC-70 using a combination of pharmacophore searching with ZINCPharmer and AutoDock Vina molecular docking. **C.C. Clement**, J. Gonzalez, M. Philipp

MEDI **470.** Bioguided fractionation and isolation of chemical constituents of the chloroform extract from the Puerto Rican plant *Simarouba tulae*. **C.A. Ospina**, P. Vivas, E. Hernandez

MEDI **471.** Synthesis of amino derivatives of dehydroleucodine and dehydroparishin-B as potential anti-proliferative against breast cancer and B16 melanoma cells. **A. Sanchez**, M. Veisaga, S.F. Wnuk, M. Barbieri, L.A. Lopez

MEDI **472.** Design and evaluation of cyclic peptides containing arginine, lysine and tryptophan residues as a cellular drug delivery system and establishing structure-activity relationship. S. Mozaffari, N. Sadeghiani, R. Tiwari, **K. Parang**

MEDI **473.** Design, synthesis and evaluation of potent inhibitors of PARP-14/ARTD8, a mono-ADP-ribosyltransferase. **M. Meyers**, **K. Upton**, A. Thorsell, H. Schuler, D. Ferraris

MEDI **474.** Design, synthesis, and evaluation of potent DNA-alkylating agents for use in Antibody-Drug Conjugates (ADCs). **K.E. Archer**, E.E. Reid, M. Shizuka, A. Wilhelm, N.C. Yoder, C. Bai, N. Fishkin, M. Bogalhas, P. Salomon, L. Harris, E.K. Maloney, O. Ab, R.V. Chari, M.L. Miller

MEDI **475.** Improved trifluoromethylation via organic electrochemistry. **J. Chen**, J. Starr

MEDI **476.** R996, an orally-bioavailable and selective activator of nuclear factor (erythroid-derived 2)-like 2 (Nrf2), is active in a Murine model of multiple sclerosis. **M.A. Duncton**, A. Owyang, F. San Pablo, A. Torneros, G. Park, D. Lau, E. Masuda, D. Payan, R. Singh

MEDI **477.** New small molecule inhibitors of Ghrelin O-acyltransferase. **J.D. Chisholm**, N.S. Mahajani, K.R. McGovern-Gooch, A. Garagozzo, A.J. Schramm, L.G. Hannah, M.A. Sieburg, J. Hougland

MEDI **478.** Fused imidazole derivatives as TGF-β inhibitors. **J. Yu**, I.S. Darwish, M. Gelman, R. Ding, A. Friera, G. Godinez, W. Lang, W. Li, K. McCaughey, J. McLaughlin, H. Nguyen, I. Smith, K. White, G. Yam, T. Kinsella, V. Taylor, S. Braselmann, C. Lamagna, E. Masuda, H. Ren, L. Chou, G. Park, R. Basile, B. Samant, D. Sweeny, M. Standlee, D. Lau, A. Torneros, F. San Pablo, G. Clemens, D. Payan, R. Singh

MEDI **479.** Fused pyrazole derivatives as TGF-β inhibitors. **I.S. Darwish**, J. Yu, M. Gelman, R. Ding, A. Friera, G. Godinez, W. Lang, W. Li, K. McCaughey, J. McLaughlin, H. Nguyen, I. Smith, K. White, G. Yam, T. Kinsella, V. Taylor, S. Braselmann, C. Lamagna, E. Masuda, H. Ren, L. Chou, G. Park, R. Basile, B. Samant, D. Sweeny, M. Standlee, D. Lau, A. Torneros, F. San Pablo, G. Clemens, D. Payan, R. Singh

MEDI **480.** Collaborative web-based architecture for fragment-based drug discovery data. **W.W. Smith**, B.A. Bunin

MEDI **481.** Planar aryl triazenes inhibit cytochrome P450 1A1 and 1B1 as a potential means to prevent cancer. **R. Nakamura**, **R. Moran**, **R.A. Isovitsch**, **D.S. Iimoto**

MEDI **482.** Discovery of BPR1K871 – a quinazoline based multi-kinase inhibitor for the treatment of AML and solid tumors: Rational design, synthesis, in vitro and in vivo evaluation. **H. Hsieh**, W. Wang, H. Shiao, Y. Ke, W. Lin, J. Hsu, C. Chen, T. Yeh

MEDI **483.** Novel approaches to the chemical synthesis of haloindoles for the development of ergot alkaloids compounds. **G. Ren**, E.J. Parish, D. Ren, Y. Lo, **H. Honda**

MEDI **484.** Novel approaches to the structure activity relationship study of citronellol type compounds useful as enzyme inhibitors. E.J. Parish, **L. Lv**, G. Ren, Y. Lo, **H. Honda**

MEDI **485.** Novel approaches to the synthetic study of lanost-8-en-3ß-ol-7,11-dione, an inhibitor of cholesterol biosynthesis. **G. Ren**, E.J. Parish, Y. Lo, **H. Honda**

MEDI **486.** Second generation inhibitors of *Porphyromonas gingivalis* biofilm formation. **F.A. Luzzio**, P.C. Patil, D.R. Demuth, J. Tan

MEDI **487.** Preparative method development from analytical columns. **J.E. Silver**, R.L. Lewis, F. Nancy, L.M. Esther

MEDI **488.** Synthesis of organic azides via flow chemistry. **J.E. Silver**, L.M. Esther, R.L. Lewis, F. Nancy

MEDI **489.** Development and screening of new cathepsin D inhibitors. **R. McConnell**, K. Malayala, K. Yarlagadda, K. Sayyar, C. Trana, W. Godwin, L. Wen

MEDI **490.** Greener reversed-phase flash chromatography using acetone instead of acetonitrile. **J.R. Bickler**

MEDI **491.** Acetonitrile as a replacement for methanol in normal-phase flash chromatography. **J.R. Bickler**

MEDI **492.** NCI/NExT discovery HTS resources: Oncology Interrogation Tools Library. **R.N. Misra**, M. Eckert, C.R. Johnson, C. Laggner

MEDI **493.** Synthesis and solubility determination of a highly water soluble phosphonooxymethyl prodrug. **R. Castillo-Bocanegra**, J. Victoria-Miguel, A. Hernandez Campos, H. Jung-Cook

MEDI **494.** Inhibition of *Candida albicans* biofilm formation with biaryl amides. **D.A. Hinojosa**

MEDI **495.** Center for innovative in drug discovery collaborative programs: Structure based drug design, synthesis and evaluation of new antischistosomal agents. **R. Tarpley**

MEDI **496.** Fragment based drug discovery of allosteric FAK inhibitors. **O. Cossio**, R. Campos-Olivas, C. Santiveri Martín-Varés

MEDI **497.** Discovery of novel small molecule inhibitors of oncoprotein EYA2 for breast and ovarian cancers. **B. Campos**, S.F. McHardy, A. Lopez, H. Wang, **D. Wilson**, **D. Wristers**, R. Li, Y. Bin, S. Smith, S. McCowen

MEDI **498.** Synthesis of N-functionalized chiral 3-hydroxyphenylpyrrolidines and their evaluation as selective D_3 receptor ligands. **A. Omran**, S. Eslamimehr, A.M. Crider, W.L. Neumann

MEDI **499.** Anti-cancer drug discovery efforts target two kinases on the non-canonical NF-κB pathway. **G. Chan**, O. Demir, G. Ghosh, R.E. Amaro

MEDI **500.** Novel mitochondrial complex I inhibitors for anti-cancer therapeutics. **J. Holmes**, K. Damera, J. Yancey, M. Zhu, N. Devi, S. Kaluz, E. Van Meir, B. Wang

MEDI **501.** Efforts to expand our antibiotic arsenal to eradicate persistent bacterial biofilms. **R. Huigens**

MEDI **502.** Design, synthesis, and biological evaluation of heteroaryl amine derivatives for anticancer activity. **M. Besan**, R. Srivastava, S. Srivastava

MEDI **503.** Luminescent Conjugated Oligothiophenes (LCOs) for detection and characterization of disease-associated protein aggregates and cells. **M. Bäck**

MEDI **504.** Drugging the undruggable with MCR scaffold manifold: The design and synthesis of covalent inhibitors and macrocycles. **T. Zarganes-Tzitzikas**, P. Patil, A. Doemling, K. Neochoritis

MEDI **505.** Synthesis of novel agents for the treatment of neurodegenerative diseases. **B.J. Eduful**, J. Leahy, D. Kang, M. Chin, A. Rashedi, O. Jallow

MEDI **506.** Withdrawn.

MEDI **507.** Artificial macrocycles by multicomponent reactions. **A. Doemling**

MEDI **508.** Cocrystal of 5-fluorouracil with nicotinamide to improve its biopharmaceutical attributes using crystal engineering approach. **M.K. Gautam**, R. Chadha

MEDI **509.** Solving challenging structural motifs in natural products using concerted DFT modeling and 2-D INADEQUATE NMR. J.R. Powell, **T.M. McCullough**, R. Iuliucci, J.K. Harper

NUCL

Division of Nuclear Chemistry and Technology

A. Hixon, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution (see *GEOC,* Wed)

Frontiers in Heavy Element Electronic Structure (see *INOR,* Wed)

Hollyweird Chemistry (see *CPRC,* Sun, Mon)

I&EC Division Early Career Fellow Symposium: Honoring Dr. Leigh Martin (see *I&EC,* Wed)

Lanthanide & Actinide Chemistry (see *INOR,* Sun, Tue, Wed, Thu)

SOCIAL EVENTS:

Social Hour, 6:00 PM: Tue

BUSINESS MEETINGS:

Executive Committee Meeting (Closed), 5:00 PM: Sun

Business Meeting, 5:00 PM: Tue

SUNDAY MORNING

Section A

Moscone Center
Esplanade Ballroom 301

Nuclear Fission

R. S. Rundberg, *Organizer*

T. A. Bredeweg, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 NUCL **1.** Total kinetic energy release and fission product mass distributions in the fast neutron induced fission of ^{235}U, ^{232}Th, ^{239}Pu and ^{233}U. **W. Loveland**

9:40 NUCL **2.** U-235 fission mass yield dependence on resonance and neutron energy. **R.S. Rundberg**, T.A. Bredeweg, M. Koehl, J. Braley

10:15 NUCL **3.** Energy dependence of fission product yields for ^{235}U, ^{238}U, and ^{239}Pu with monoenergetic neutrons between thermal and 14.8 MeV. **M. Gooden**, T.A. Bredeweg, M.M. Fowler, D.J. Vieira, J. Wilhelmy, A. Tonchev, M.A. Stoyer, M. Bhike, F. Krishichayan, W. Tornow

10:50 Intermission.

11:10 NUCL **4.** Theory of fission-fragment angular distributions. **W. Younes**

11:45 NUCL **5.** Survival of excited nuclei produced in warm fusion reactions. **C.M. Folden**

‡ *Cooperative Cosponsorship*

SUNDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 302

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Cosponsored by INOR and PRES

B. E. Bursten, W. J. Evans, A. P. Sattelberger, *Organizers*

J. C. Green, *Presiding*

1:20 NUCL **6. Award Address** (Glenn T. Seaborg Award for Nuclear Chemistry sponsored by the ACS Division of Nuclear Chemistry & Technology). Bonding trends across the actinide series. **D.L. Clark**

2:00 NUCL **7.** Some bits and pieces of Dave Clark 5d and 5f chemistry. **B.E. Bursten**

2:20 NUCL **8.** Technetium oxide chemistry. **A.P. Sattelberger**, B. Childs, K.V. Lawler, F. Poineau, P. Forster, K. Czerwinski

2:40 NUCL **9.** Recent advances in the chemistry of the rare-earth metals in the formal +2 oxidation state. **W.J. Evans**

3:00 NUCL **10.** New divalent manganese complexes supported by imine-amide ligands. **J.C. Gordon**, D. Kindra, B. Scott, N.C. Smythe

3:20 Intermission.

3:40 NUCL **11.** Uranium (IV -VI) imido and amido chemistry: Synthesis, reactivity and bonding. **J.M. Boncella**, A.M. Tondreau, N.C. Tomson, N.H. Anderson, B. Scott

4:00 NUCL **12.** Structural chemistry of UO_2, NpO_2, and PuO_2. **S. Conradson**

4:20 NUCL **13.** Reactivity of +3 actinides. **S.A. Kozimor**, E.R. Batista, J.M. Berg, E.R. Birnbaum, J.N. Cross, J.W. Engle, J. Pacheco, M.G. Ferrier, B.W. Stein

4:40 NUCL **14.** Actinide coordination chemistry with environmental and biological applications. **M. Neu**

5:00 NUCL **15.** Actinide organometallic chemistry: A meeting with David Clark at the bottom of the periodic table. **J.L. Kiplinger**

Section B

Moscone Center

Esplanade Ballroom 301

Nuclear Fission

T. A. Bredeweg, *Organizer*

R. S. Rundberg, *Organizer, Presiding*

2:00 Introductory Remarks.

2:05 NUCL **16.** Fission yield measurements for Th-232, U-238 and HEU at the National Ignition Facility. **N. Gharibyan**, K. Moody, J. Despotopulos, S. Faye, P. Grant, K. Kmak, K. Roberts, C. Yeamans, D.A. Shaughnessy

2:40 NUCL **17.** Application of the Bohr-independence hypothesis for the measurement of fission yields. **N. Gharibyan**, K. Moody, S. Tumey, T. Brown, D.A. Shaughnessy

3:15 Intermission.

3:35 NUCL **18.** Addressing nuclear data needs with FIER. **E. Matthews**, B.L. Goldblum, W. Younes, L.A. Bernstein

4:10 NUCL **19.** Delayed neutron spectroscopy for characterization of special nuclear material. J. Ocampo, J. Wallick, G.E. Miller, **A. Shaka**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 302

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Cosponsored by INOR

B. E. Bursten, W. J. Evans, A. P. Sattelberger, *Organizers*

D. K. Shuh, *Presiding*

8:20 NUCL **20.** Tribute to an esteemed colleague: Young Doctor Clark. **D.E. Hobart**

8:40 NUCL **21.** Coordination of N-heterocyclic ligands to actinides: A joint theoretical and experimental study. **P. Yang**, J. Su, E.R. Batista, J.K. Gibson, A. Gaunt, S.A. Kozimor

9:00 NUCL **22.** Probing actinide-ligand chemical bonds: Hand shake between quantum mechanical calculations and experimental measurements. **E.R. Batista**, P. Yang, R.L. Martin, S.A. Kozimor, D.L. Clark

9:20 NUCL **23.** Interpretation of morphologic and chemical signatures from actinide oxide materials. **M.P. Wilkerson**

9:40 NUCL **24.** Withdrawn.

10:00 NUCL **25.** Factors affecting the sorption of uranyl at mineral-aqueous solution interfaces. **G.E. Brown**, G. Dublet, V. Noel, S.E. Fendorf, J.R. Bargar, K. Maher

10:20 Intermission.

10:40 NUCL **26.** Molecular controls over uranium mobility in complex redox-active sediment systems. **J.R. Bargar**, V. Noël, S. Bone, N. Janot, S. Roycroft, K. Boye

11:00 NUCL **27.** Swift heavy ion irradiation of actinide materials. **R. Ewing**

11:20 NUCL **28.** Synthesis, structure and bonding of tetravalent-metal (M^{IV}) oxide clusters. **L. Soderholm**, S. Skanthakumar, S.L. Estes

11:40 NUCL **29.** Covalent interactions in actinide oxides. **P.S. Bagus**, C.J. Nelin

Section B

Moscone Center

Esplanade Ballroom 301

Nuclear & Radiochemistry Summer School: Past, Present & Future

J. D. Robertson, *Organizer*

D. D. Ensor, *Organizer, Presiding*

8:20 Introductory Remarks.

8:30 NUCL **30.** Impact of the nuclear and radiochemistry summer schools on the nuclear chemistry program at Michigan State University. **P.F. Mantica**

8:55 NUCL **31.** How the Nuclear and Radiochemistry Summer School shaped my career as a radiochemist in biotech. **C.A. Boswell**

9:20 NUCL **32.** My career in nuclear science: From the nuclear and radiochemistry summer school to national security. **J. Freiderich**

9:45 NUCL **33.** Nuclear science from the big apple to down under. **R. Popelka-Filcoff**

10:10 Intermission.

10:25 NUCL **34.** Structural and chemical changes in uranyl fluoride: A complementary spectroscopic and computational study. **M.C. Kirkegaard**, A.J. Miskowiec, J. Langford, B. Anderson

10:50 NUCL **35.** Path to a PhD: From a summer to a career. **A.J. Swift**, K. Czerwinski, D.J. Koury

11:15 NUCL **36.** Finding my place in radiochemistry: A recent grad's letter of gratitude to the NCSS. **E.M. May**

11:40 NUCL **37.** Impact of the Nuclear Chemistry Summer School on one student from a small, undergraduate liberal arts college. **A. Klose**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 302

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Cosponsored by INOR

B. E. Bursten, W. J. Evans, A. P. Sattelberger, *Organizers*

C. Burns, *Presiding*

1:40 NUCL **38.** Coordination chemistry of uranium with thioethers and selenoethers: Investigation of neutral heavy donor binding to heavy metals. A.V. Blake, Z. Theiler, **S.R. Daly**

2:00 NUCL **39.** Harnessing the principles of coordination chemistry to control the growth of actinide materials. **S.G. Minasian**, A. Herve, A. Braun, S. Alayoglu, A.B. Altman, C. Booth, D. Olive

2:20 NUCL **40.** C-term magnetic circular dichroism spectroscopy: From transition metals to f-element chemistry. **M.L. Neidig**

2:40 NUCL **41.** Synchrotron radiation for the investigation of heavy element science. **D.K. Shuh**

3:00 NUCL **42.** Activation of uranyl in gas-phase complexes. **J.K. Gibson**

3:20 Intermission.

3:40 NUCL **43.** Separating technetium from nitric acid by trapping in iron oxides. **W.W. Lukens**

4:00 NUCL **44.** Water adsorption on AnO_2 (An = U, Pu) surfaces. J. Wellington, B. Tegner, A. Kerridge, **N. Kaltsoyannis**

4:20 NUCL **45.** Electronic structures and photoelectron spectra of uranium halides and oxides. J. Su, L. Wang, **J. Li**

4:40 NUCL **46.** Broadening student experiences: Research internships with Los Alamos National Laboratory and the interesting Pu chemistry they performed. **P.K. Dorhout**

5:00 NUCL **47.** Realizing cerium(IV)-ligand multiple bonds: Cerium is a 5d element after all? **E.J. Schelter**, L. Solola, A. Zabula, W.L. Dorfner, B. Manor, P. Carroll

Section B

Moscone Center

Esplanade Ballroom 301

Nuclear & Radiochemistry Summer School: Past, Present & Future

D. D. Ensor, *Organizer*

J. D. Robertson, *Organizer, Presiding*

1:20 NUCL **48.** Heavy actinide thermodynamics: Research enabled by the Nuclear Chemistry Summer School. **J. Braley**, M. Luckey, M. Urban, N. Bessen

1:45 NUCL **49.** Radiochemistry Center of Excellence and the NCSS: To infinity and beyond. **J.D. Auxier**, M.T. Cook, M. Lang, D.C. Donovan, H.L. Hall

2:10 NUCL **50.** From Brookhaven to the Bronx: Radiochemistry and education. **M.A. Deri**

2:35 NUCL **51.** NCSS to doctoral candidate: Determination of radioisotopes in complex saline matrices. **J.K. Daum**, R. Sudowe

3:00 Intermission.

3:15 NUCL **52.** Education blended with inspiration: Nuclear chemistry summer schools. **A.L. Werlein**

3:40 NUCL **53.** Thermodynamic analysis of lanthanide halides and oxyhalides. **D. Miller**, J.D. Auxier, H.L. Hall

4:05 NUCL **54.** From the summer school to graduate school: Leveraging opportunities in nuclear chemistry. **R. Lewis**

4:30 NUCL **55.** Nuclear and radiochemistry summer school: (Almost) six years later. **J.M. Dorhout**

4:55 NUCL **56.** 2016 Class of the DOE Radiochemistry Summer School in Oregon State University. **A. Paulenova**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

TUESDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 302

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Cosponsored by INOR

B. E. Bursten, W. J. Evans, A. P. Sattelberger, *Organizers*

A. Kersting, *Presiding*

8:20 NUCL **57.** Development of actinide separations in alkaline solutions. **G. Jarvinen**, W.H. Runde, G. Goff

8:40 NUCL **58.** Subsurface containment and permanent disposal of nuclear waste: Role and contribution of fundamental actinide science. **D.T. Reed**

9:00 NUCL **59.** Recent progress in studies of internuclear interactions in heavy element systems by solid-state NMR and NQR spectroscopy. **H. Cho**, C. Capan, R. Dempsey, B.K. McNamara, S. Sinkov, C. Soderquist

9:20 NUCL **60.** Amplification in late actinides: How the minor nuances of electronic structure create bulk effects. **T.E. Albrecht-Schmitt**

9:40 NUCL **61.** Differential solvation effects on reaction energetics. **G. Schreckenbach**

10:00 NUCL **62.** Actinide-sulfilimine chemistry. **J.R. Walensky**

10:20 Intermission.

10:40 NUCL **63.** Preparation and reactivity of the $[Re_2F_8]^{2-}$ anion. **F. Poineau**, S. Mariappan Balasekaran, A.P. Sattelberger

11:00 NUCL **64.** Thorium redox chemistry and a new way to measure actinide covalency by pulsed EPR spectroscopy. **D. Mills**, E. McInnes, F. Tuna, A. Kerridge, L. Maron, A. Formanuik, A. Ariciu, F. Ortu, J. Liu, R. Beekmeyer, L. Castro

11:20 NUCL **65.** Structures and phase transitions of the actinide hexachlorides. **R. Wilson**

11:40 NUCL **66.** Why does solid PuO_2 possess no magnetic moment? **R.L. Martin**

Section B

Moscone Center

Esplanade Ballroom 301

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Cosponsored by INOR and PRES

D. L. Clark, D. K. Shuh, L. Soderholm, *Organizers*

C. Burns, *Presiding*

8:20 NUCL **67.** Electronic structures of F_3UAH (A = C - Fl) molecules: Lewis Electron-Pair (LEP) model revisited. H. Hu, W. Li, **J. Li**

8:40 NUCL **68.** Experimental and computational study of protactinium, the transition metals and the actinides. **R. Wilson**, V. Vallet

9:00 NUCL **69.** Still thoroughly modern at 25: The FEUDAL bonding model. **J.L. Sonnenberg**

9:20 NUCL **70.** Magic journey in metal-metal multiple bonds. **L. Gagliardi**

9:40 NUCL **71.** Covalency in 4f-element complexes probed with quantum mechanics and ligand K-edge x-ray absorption spectroscopy. **E.R. Batista**, P. Yang, R.L. Martin, S.A. Kozimor, D.L. Clark

10:00 Intermission.

10:20 NUCL **72.** Theory enables soft x-ray synchrotron radiation spectroscopy of heavy element materials. **D.K. Shuh**

10:40 NUCL **73.** Photoelectron spectroscopy and density functional theory: The interplay of experiment and theory. **J.C. Green**

11:00 NUCL **74.** Stabilities of actinide oxidation states in gas-phase complexes. **J.K. Gibson**

11:20 NUCL **75.** Complexation of Am^{3+}, Cm^{3+}, Bk^{3+} and Cf^{3+} with DPA ligand in water: A theoretical study. **P. Yang**, M. Kelley, E.R. Batista, J. Braley

11:40 NUCL **76.** Taking advantage of the chemistry of heterocycles in actinide coordination: Crystal packing, reactivity, and pi-pi interactions of nitrogen donor ligands containing naphthalene and phenazine. **A.E. Gorden**, E.E. Hardy, K.M. Wyss, M.A. Eddy, R.J. Keller

TUESDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 302

Glenn T. Seaborg Award for Nuclear Chemistry: Symposium in honor of David L. Clark

Cosponsored by INOR

B. E. Bursten, W. J. Evans, A. P. Sattelberger, *Organizers*

J. C. Gordon, *Presiding*

1:40 NUCL **77.** Unique advantages of organometallic supporting ligands. **P. Diaconescu**

2:00 NUCL **78.** Complexes of uranium and thorium with multiple bonds to tetryl and pnictide centers. **S.T. Liddle**, J. Seed, M. Gregson, A. Wooles, F. Tuna, E. McInnes

2:20 NUCL **79.** Synthesis and x-ray crystallographic characterization of low valent organoplutonium complexes: Identification of plutonium in the +2 oxidation state. **C.J. Windorff**, B. Scott, A. Gaunt, S.A. Kozimor, W.J. Evans

2:40 NUCL **80.** Pushing the limits with f element-ligand multiple bonding. **T.W. Hayton**

3:00 NUCL **81.** Mediating redox chemistry at the lanthanides using redox-active ligands. S.A. Pattenaude, E.J. Coughlin, M. Zeller, **S.C. Bart**

3:20 Intermission.

3:40 NUCL **82.** Electrocatalytic production H_2 from H_2O with f-element-based molecular catalysts. **K. Meyer**

4:00 NUCL **83.** Evaluation of mixed actinide oxides by laser ablation ICP-MS. K. Campbell, A. Unger, W.M. Kerlin, T. Hartmann, J. Bertoia, E. Judge, M. Dirmyer, **K. Czerwinski**

4:20 NUCL **84.** Computational study of semiconducting layered technetium chalcogenide compounds. **E. Kim**, P. Weck, F. Poineau, A.P. Sattelberger, K. Czerwinski

4:40 NUCL **85.** Computational studies of hydrolysis reactions of cationic and anionic actinide complexes. **D.A. Dixon**, M. Vasiliu, H. Arnold, K.A. Peterson, J.K. Gibson

Section B

Moscone Center

Esplanade Ballroom 301

Frontiers in Heavy Element Electronic Structure: A Tribute to Bruce Bursten

Cosponsored by INOR and PRES

D. L. Clark, L. Soderholm, *Organizers*

D. K. Shuh, *Organizer, Presiding*

1:20 NUCL **86.** Calculating fellow: A theoretical tribute to Bruce Bursten. **D.E. Hobart**

1:40 NUCL **87.** Energetic properties of actinide molecular clusters. **D.A. Dixon**, M. Vasiliu, Z. Lee

2:00 NUCL **88.** Layered metal oxide nanosheets as model surfaces for understanding the strong metal-support interaction. M. Strayer, A.S. Rosas, R. Uppuluri, J.M. Binz, T. Senftle, A. Azizi, R.M. Rioux, M.J. Janik, N. Alem, **T.E. Mallouk**

2:20 NUCL **89.** Shortest Th–Th distance from a new type of quadruple bond. H. Hu, **N. Kaltsoyannis**

2:40 NUCL **90.** Actinide-pnictogen chemistry. **J.R. Walensky**

3:00 Intermission.

3:20 NUCL **91.** Accurate solution phase thermochemistry for actinide solvation, complexation, and transport from aqueous to organic phases. **A.E. Clark**

3:40 NUCL **92.** From actinides to transactinides: Peculiarities in electronic structure and properties. **V. Pershina**

4:00 NUCL **93.** Roles of 4f and 5f orbitals in bonding: A magnetochemical, crystal field, density functional theory, and multi-reference wavefunction study. **W.W. Lukens**, M. Speldrich, P. Yang, T. Duignan, J. Autschbach, P. Koegerler

4:20 NUCL **94.** Insights into the redox chemistry of actinides. **W. Dejong**

4:40 NUCL **95.** New insights into metal-ion correlations in solution. **L. Soderholm**, S. Skanthakumar

WEDNESDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 302

Advanced Actinide Materials: Nanostructure, Complexity & Extreme Environments

P. C. Burns, G. Sigmon, *Organizers*, *Presiding*

8:30 NUCL **96.** Updates on uranyl peroxide nanoclusters. **P.C. Burns**

9:00 NUCL **97.** Dissolution of uranium minerals in uranyl peroxide nanocluster forming environments. **H.L. Lobeck**, C.J. Parker, S. Boukdad, E. Balboni, P.C. Burns

9:20 NUCL **98.** Structural stability of uranyl nanoclusters. **M. Sharifironizi**, J. Qiu, J. Szymanowski, P.C. Burns

9:40 NUCL **99.** Sorption mechanism and kinetics of the uranyl peroxide nanocluster (U60) to Ca-and Na-montmorillonite. **L.R. Sadergaski**, W. Stoxen, A.E. Hixon

10:00 Intermission.

10:15 NUCL **100.** Uranyl polyrotaxanes: From hydrothermal synthesis to structural diversity. **W. Shi**

10:45 NUCL **101.** Actinide based metal organic framework materials. **S. Wang**

11:05 NUCL **102.** Effect of processing conditions on lanthanide and actinide oxalate crystal growth mechanisms: Insights from in situ characterization and computational modeling. **J.A. Soltis**, M. Conroy, W.C. Isley, T. Meadows, T. Meadows, G.B. Hall, S. Chatterjee, Z. Wang, S. Kathmann, J.J. De Yoreo, E. Buck, G.J. Lumetta

11:25 NUCL **103.** Formation and growth mechanism of U(IV) nanoparticles and colloidal stability in aqueous solutions. **W. Cha**, H. Cho, Y. Youn, E. Jung

Section B

Moscone Center

Esplanade Ballroom 301

General Topics in Nuclear Chemistry & Technology

L. H. Delmau, *Organizer, Presiding*

8:30 NUCL **104.** Withdrawn.

8:50 NUCL **105.** Cyclic voltammetric studies of unique complexation and solvent effects for the actinide elements. **M.L. Marsh**, F.D. White, D.E. Hobart, S.S. Galley, T.E. Albrecht-Schmitt

9:10 NUCL **106.** Investigation of structure and bonding in transuranium elements utilizing a redox active ligand. **S.S. Galley**, S.A. Pattenaude, S.C. Bart, T.E. Albrecht-Schmitt

9:30 NUCL **107.** Unraveling the nature of the Am(III)/Eu(III) separation with three structurally similar ligands by changing of bridging groups. **Q. Wu**

9:50 Intermission.

10:10 NUCL **108.** Chemistry of technetium in dilute to concentrated saline systems: Redox processes, solubility and complexation. X. Gaona, **E. Yalcintas**, A. Baumann, R. Polly, M. Altmaier, H. Geckeis

10:30 NUCL **109.** Redox behavior of U(VI)/U(IV) and solubility of U(IV) in repository relevant dilute to concentrated solutions in the absence and presence of complexing ligands. **E. Yalcintas**, N. Cevirim, X. Gaona, D.T. Reed, M. Altmaier

10:50 NUCL **110.** Complexation of lanthanide and actinide ions with N,N-di-2-ethylhexyl-diglycol-amic acid in solvent extraction separation from nitric acid solutions. **G. Tian**, Y. Zhang, S. Yang, X. Yuan

11:10 NUCL **111.** Effect of elevated temperatures on actinide solubility and speciation–studies performed by KIT-INE within the German project ThermAc. X. Gaona, F. Endrizzi, J. Lee, **D. Fellhauer**, M. Altmaier

11:30 NUCL **112.** Complexation and phase transfer kinetics of tributyl phosphate degradation products at the liquid:liquid interface during solvent extraction. **S. Howett**, A. Casella, A. Lines, S. Clark, C. Louie, C. Delegard, G.J. Lumetta, W. Pitts, K.M. McCoy

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

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Frontiers in Heavy Element Electronic Structure

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Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

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WEDNESDAY AFTERNOON

Section A

Moscone Center
Esplanade Ballroom 302

Advanced Actinide Materials: Nanostructure, Complexity & Extreme Environments

P. C. Burns, G. Sigmon, *Organizers*, *Presiding*

1:00 NUCL **113.** Effects of high ionic strength on actinide speciation and oxidation state distribution in subsurface environments. **D.T. Reed**, M.K. Richmann, J.S. Swanson, T. Dittrich

1:30 NUCL **114.** Corrosion mechanism of iron in liquid uranium hexafluoride environment. **M. Achour**, M. Dubois, L. Jouffret, A. Selmi, B. Morel, S. Delpech, S. Chatain, L. Martinelli, P. Bonnet

1:50 NUCL **115.** Turning on the terminal: Promoting non-covalent interaction with uranyl oxo atoms. **K. Carter**, M. Kalaj, R. Surbella, L. Ducati, J. Autschbach, C.L. Cahill

2:10 NUCL **116.** Insight into the uranyl oxyfluoride topologies through the synthesis and crystal structure new oxyfluoride compounds. **L. Jouffret**, J. Hiltbrunner, M. Dubois

2:30 Intermission.

2:45 NUCL **117.** Actinide clusters, nanoclusters and cluster-frameworks. C. Falaise, K. Kozma, O. Renier, H.A. Neal, **M.D. Nyman**

3:15 NUCL **118.** Influence of alkali metals in dissolving UO_2 to form highly soluble aqueous uranyl peroxide clusters. **S. Hickam**, P.C. Burns

3:35 NUCL **119.** Uranyl-peroxide nanocapsules: From self-assembly to isomerism. **P. Miro**

3:55 NUCL **120.** Thermochemistry of neptunium oxides and Np incorporated studtite. **L. Zhang**, E. Dzik, J. Szymanowski, G. Sigmon, A. Navrotsky, P.C. Burns

4:15 NUCL **121.** Plutonium nanocluster formation, structure, and stability. **A.E. Hixon**, G. Sigmon

Section B

Moscone Center
Esplanade Ballroom 301

General Topics in Nuclear Chemistry & Technology

L. H. Delmau, *Organizer, Presiding*

1:20 NUCL **122.** Developing regional isotopic baselines to trace resource acquisition patterns in the Mesa Verde area of the American Southwest. **A.L. Werlein**, V. Renson, J. Coltrain, K. Schollmeyer, J.D. Robertson, J.R. Ferguson

1:40 NUCL **123.** Characterization of indigenous Australian ochre by k_0-Neutron Activation Analysis (k_0-NAA) for understanding cultural exchange. **R. Popelka-Filcoff**, C. Lenehan, J. Bennett, A. Stopic, K. Walshe

2:00 NUCL **124.** $^{88}Zr(n,\beta)^{89}Zr$ cross section measurement. **J. Shusterman**, J.M. Gates, S.E. Lapi, C.S. Loveless, E.B. Norman, G. Peaslee, J.D. Robertson, G. Severin, L. Sutherlin, K.J. Thomas, M.A. Stoyer, D.A. Shaughnessy, N.D. Scielzo

2:20 NUCL **125.** Another isomer in Rh102? H.A. Shugart, K.J. Thomas, **E.B. Norman**

2:40 Intermission.

3:00 NUCL **126.** Unusual coordination of heptadentate tripodal Schiff base lanthanide/actinide complexes. **K. Seidler**

3:20 NUCL **127.** Utility of MOFs and their derivatives for luminescent sensing and sorption of actinide ions from aqueous solution. **L. Yuan**, N. Zhang, Z. Chai, W. Shi

3:40 NUCL **128.** Ion selectivity of uranyl peroxide nanocages: An inorganic mimic of K^+ ion channels. **Y. Gao**, J. Szymanowski, X. Sun, P.C. Burns, T. Liu

4:00 NUCL **129.** Possible atomic fuel production through accumulation of specific radioisotopes by fish in offshore Fukushima, Japan. **H. Katsura**

4:20 NUCL **130.** Thermodynamic studies on the complexation of uranyl ion in ionic liquids. **C. Xu**, J. Chen

Evolving Nanoparticle Reactivity throughout Nucleation, Growth & Dissolution

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Frontiers in Heavy Element Electronic Structure

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WEDNESDAY EVENING

Section A

Moscone Center
Hall D

General Topics in Nuclear Chemistry & Technology

A. E. Hixon, *Organizer*

7:00 - 9:00

NUCL **131.** Determination of radioactivity of uranium and thorium in environmental samples by using fusion and sequential separation method, and its evaluation using key validation parameters. **Y. Ko**, W. Kim, H. Kim, W. Lee, G. Choi, K. Chung, M. Kang

NUCL **132.** Modeling redox coordination chemistry for transuranium elements. **F.D. White**, M.L. Marsh, S.S. Galley, D.E. Hobart, T.E. Albrecht-Schmitt

NUCL **133.** Preparation of alumina microspheres by internal gelation method. **C. Padilla-Cintron**, J. Katalenich

NUCL **134.** Characterization of lanthanide chlorides for nuclear forensics. **S. Shahbazi**, J. Auxier

NUCL **135.** Synthesis of Bis-Triazinyl Pyridine (BTPs) ligands for ^{15}N ESEEM experiments in actinide and lanthanide complexes. **D. Dan**, T.E. Albrecht-Schmitt

NUCL **136.** PDF analysis of uranyl clusters from aqueous solutions. **K. Kozma**, C. Falaise, H.A. Neal, M.D. Nyman

NUCL **137.** Ordered mesoporous carbons functionalized for actinide and lanthanide separations chemistry. **K. Kluherz**, G. Deodhar, E. Bertelsen, J. Braley, B.G. Trewyn

NUCL **138.** Soft N-, S-, and mixed donor site ligands for selective separation of actinides from lanthanides. **M. Twomey**, **I. Lehman-Andino**, L. Mathivathanan, R.G. Raptis, K. Kavallieratos

NUCL **139.** Electrochemical reduction of aqueous uranium. **B. Stevenson**, J. Scaggs, D.D. Russell

THURSDAY MORNING

Section A

Moscone Center
Esplanade Ballroom 302

Young Investigators in Nuclear & Radiochemistry

Cosponsored by YCC

A. E. Hixon, *Organizer*

E. M. May, *Organizer, Presiding*

8:30 NUCL **140.** Re (III and V) Schiff base complexes as potential therapeutic agents. **J.E. Baumeister**, C. Barnes, S.S. Jurisson

8:50 NUCL **141.** Radiolabeling of a trithiol-bombesin ligand with ^{77}As and ^{72}as for use as radiopharmaceuticals. **M. Phipps**, Y. Feng, F. Gallazzi, A. Ketring, S.S. Jurisson

9:10 NUCL **142.** Application of inductively coupled plasma mass spectroscopy and enriched tungsten isotopes to nuclear fusion research. **J. Duran**, D.C. Donovan, C. Eley, A. Maan, J.D. Auxier, S. Lee, S. Zamperini, E. Unterberg, D. Rudakov, P. Stangeby, W. Wampler

9:30 NUCL **143.** Actinide-carbon bond activation in gas-phase organoactinide complexes. **J. Jian**, T. Eaton, J.K. Gibson

9:50 NUCL **144.** Characterizing actinide speciation using electrospray ionization mass spectrometry. **T. Eaton**, J. Jian, J.K. Gibson

10:10 Intermission.

10:30 NUCL **145.** Utilizing Diffusion Ordered Spectroscopy (DOSY) to probe organic phases in liquid-liquid solvent extraction systems. **A. Kimberlin**, K.L. Nash

10:50 NUCL **146.** Study of actinide cations in solution through their paramagnetic behavior. **M. Illy**, M. Autillo, L. Guerin, D. Guillaumont, E. Colineau, P. Moisy, H. Bolvin, C. Berthon

11:10 NUCL **147.** Method comparison for the determination of Pitzer parameters for Tc(VII), Re(VII), and V(V) in aqueous systems. C. Eiroa Lledo, **G. Parker**, D.E. Wall, N. Wall

11:30 NUCL **148.** Elucidating bonding preference in tetrakis(imido)urinate (VI) dianions. **J. Xie**, N.H. Anderson, D. Ray, M. Zeller, S.C. Bart, L. Gagliardi

Section B

Moscone Center
Esplanade Ballroom 301

General Topics in Nuclear Chemistry & Technology

L. H. Delmau, *Organizer*

A. E. Hixon, *Presiding*

8:20 NUCL **149.** Radiochemical, elemental, and isotopic analysis of epsilon phase material from irradiated fuel. **K.L. Pellegrini**, C. Soderquist, R.A. Clark, J.M. Schwantes

8:40 NUCL **150.** Microstructural examination of neutron irradiated base metal and TIG-welded zircaloy-4. **C. Silva**, K. Leonard, C. Bryan

9:00 NUCL **151.** Using technetium's volatility to decontaminate barrier material. **W.R. Wilmarth**, L. Oji, M. Restivo, M. Duignan

9:20 NUCL **152.** Semiconductivity in plutonium and americium chromates and molybdates: Evidence for energy-degeneracy-driven covalency. **A. Arico**

9:40 NUCL **153.** Recent progress on the development of pyroprocessing techniques for TMSR in SINAP. **Y. Gong**, Q. Li

10:00 Intermission.

10:20 NUCL **154.** Pyroprocessing of spent nuclear fuels: Theoretical calculations and multiscale molecular simulations of solute behavior in molten salts. **X. Li**, L. Yan, J. Song, S. Shi, B. Yue

10:40 NUCL **155.** Speciation of uranium in condensing laser ablation plasmas. **D. Weisz**, J.C. Crowhurst, H. Radousky, T. Rose, W. Siekhaus, B. Koroglu, M. Armstrong, E. Stavrou, J.M. Zaug, M. Azer, M. Finko, D. Curreli

11:00 NUCL **156.** Design and efficient synthesis of a bifunctional octadentate ligand for PET imaging with ^{89}Zr. **M.A. Abdalrahman**, R.P. Planalp

11:20 NUCL **157.** Contamination and decontamination of steel components. **A. Lang**, D. Engelberg, P. Coffey, P. Martin, N. Smith, A. Jenkins, G. Law

11:40 NUCL **158.** Automated clean chemistry for bulk analysis of environmental swipe samples. **S.C. Bottorff**, K.N. Tevepaugh, D.A. Bostick, C.R. Hexel, H. Kim, P. Field, B.W. Ticknor

THURSDAY AFTERNOON

Section A

Moscone Center
Esplanade Ballroom 302

Young Investigators in Nuclear & Radiochemistry

Cosponsored by YCC

E. M. May, *Organizer*

A. E. Hixon, *Organizer, Presiding*

1:30 NUCL **159.** Characterizing mixed ligand f-element complexes for better An(III)/Ln(III) separations. **I.M. Hobbs**, K.L. Nash

1:50 NUCL **160.** Studies of the impact of the diluent on interfacial properties of the advanced TALSPEAK/ALSEP extractant HEH[EHP]. **D.E. Dodd**, K.L. Nash

2:10 NUCL **161.** Liquid phase chemistry study of indium and thallium for a future investigation of element 113. **M.F. Volia**, E. Tereshatov, M. Boltoeva, C.M. Folden

2:30 NUCL **162.** Environmental technetium chemistry: Sulfide treatment of iron-containing minerals. K. Reinig, **N. Moore**, S.S. Jurisson, T. Phelps

2:50 NUCL **163.** Withdrawn.

3:10 Intermission.

3:30 NUCL **164.** Europium sorption to aluminum (hydr)oxide minerals. **P. Kay**, T. Baumer, A.E. Hixon

3:50 NUCL **165.** Alkali ion bridge complexation between uranium nanoclusters and mineral surfaces. **W. Stoxen**, L.R. Sadergaski, J. Szymanowski, A.E. Hixon

4:10 NUCL **166.** Determination of thermodynamic parameters associated with Tc(IV) sulfate complexation. **G. Parker**, D.E. Wall, N. Wall

4:30 NUCL **167.** Stability of uranyl peroxide nanoclusters under hydrothermal conditions. **J.R. FitzPatrick**, H.L. Lobeck, S. Mana, P.C. Burns

ORGN

Division of Organic Chemistry

R. Broene and S. Silverman, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Advances in Teaching Organic Chemistry (see *CHED,* Tue)

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors (see *ENVR,* Tue)

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium (see *PROF,* Sun, Mon)

Organometallic Chemistry: Applications to Organic Transformations (see *INOR,* Sun, Wed)

Space Chemistry (see *YCC,* Mon)

SOCIAL EVENTS:

Social Hour, 8:30 PM: Wed

SUNDAY MORNING

Section A

Moscone Center
3018/3022

George A. Olah Award in Hydrocarbon or Petroleum Chemistry: Symposium in honor of Robert H. Grubbs

R. E. Maleczka, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN **1.** Metal-catalyzed cross-coupling reactions of alkyl electrophiles. **G.C. Fu**

8:40 ORGN **2.** Catalytic C–H functionalization: Borylation of molecules great and small along the road out of Flatland. **M.R. Smith**

9:15 ORGN **3.** Streamlined synthesis of π-systems containing antiaromatic cyclobutadienoids via C-H activated annulation and aromatization. **Y. Xia**

9:50 Intermission.

10:00 ORGN **4.** Organocatalyzed atom transfer radical polymerization driven by visible light. **G. Miyake**

10:35 ORGN **5.** Synthesis of improved protein-polymer conjugates by ROMP and CRP. **H.D. Maynard**

11:10 ORGN **6. Award Address** (George A. Olah Award in Hydrocarbon or Petroleum Chemistry sponsored by the George A. Olah Award Endowment). Selective olefin metathesis catalysts and their applications. **R.H. Grubbs**

11:55 Concluding Remarks.

Section B

Moscone Center
3014/3016

National Fresenius Award: Symposium in honor of Neal K. Devaraj

Cosponsored by BIOL

Financially supported by Phi Lambda Upsilon, the National Chemistry Honor Society

E. M. Skoda, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN **7.** Design and synthesis of new chemical tools for probing, manipulating, and imaging biological systems. **D.M. Chenoweth**

8:45 ORGN **8.** Regio- and chemoselective immobilization of proteins on surfaces. J. Seo, G. Ramamoorthy, **C.D. Poulter**

9:25 ORGN **9.** Membrane architectures, vesicle and viral fusion using DNA-lipid conjugates. **S.G. Boxer**

10:05 Intermission.

10:20 ORGN **10.** Purposefully moving peptides and proteins into the cytosol. **A. Schepartz**

11:00 Introduction of Awardee.

11:05 ORGN **11. Award Address** (National Fresenius Award sponsored by the Phi Lambda Upsilon, The National Chemistry Honor Society). Novel coupling reactions for manipulating and imaging biomolecules. **N.K. Devaraj**

11:55 Concluding Remarks.

Section C

Moscone Center
3011

Biologically-Related Molecules & Processes

R. D. Broene, *Organizer*

S. T. Handy, *Presiding*

8:20 ORGN **12.** Aurones: Synthesis and a template for biological investigations. **S.T. Handy**

8:40 ORGN **13.** Versatile synthesis of chlorin and application in bio-medicine. **N. Bhupathiraju**, J. Gonzales, W. Perea, H. Chu, M. Yuen, N.L. Greenbaum, C.M. Drain

9:00 ORGN **14.** Structural modifications of OXE receptor antagonists towards improved *in vivo* metabolic stability. **S. Chourey**, Q. Ye, .N. Reddy, R. Wang, S. Gravel, C. Cossette, I. Slobodchikova, D. Vuckovic, M. Zeller, W.S. Powell, J. Rokach

9:20 ORGN **15.** Fluorescent probes for imaging potassium in living cells. **Z. Wang**

9:40 ORGN **16.** Fluorogenic dyes for haloalkane-based protein labeling *in vitro* and in bacterial cells. **S.A. Clark**, V. Singh, D. Vega Mendoza, W. Margolin, E.T. Kool

10:00 ORGN **17.** Hydrophilized cell-permeant dyes with secondary alcohol functionalities for live cell STED imaging. **A.N. Butkevich**, V.N. Belov, K. Kolmakov, G. Lukinavicius, D. Kamin, S.C. Sidenstein, J. Matthias, R. Vlijm, H. Shojaei, V.V. Sokolov, S.W. Hell

10:20 ORGN **18.** Design of a novel fluorescent sensor for chloride. **K. VanDenburgh**, Y. Liu, B. Qiao, A.H. Flood

10:40 ORGN **19.** Fluorescent probes for imaging formaldehyde in living cells. **K.J. Bruemmer**, R.R. Walvoord, T.F. Brewer, C.J. Chang

11:00 ORGN **20.** Development of a practical synthesis of ERK inhibitor GDC-0994. **N. Wong**, X. Linghu, F. Gosselin

11:20 ORGN **21.** Discovery chemistry towards BTK inhibitor GDC-0853. **J.J. Crawford**

11:40 ORGN **22.** Process research and development of the commercial synthesis of BTK inhibitor GDC-0853. **H. Zhang**, T. Cravillion, Q. Tian, N. Lim, D. Beaudry, J. Defreese, F. Gosselin

Section D

Moscone Center
3009

Asymmetric Reactions & Syntheses

R. D. Broene, *Organizer*

D. K. Leahy, *Presiding*

8:00 ORGN **23.** Organocatalytic asymmetric transfer hydrogenation of *N*-alkylated aryliminoesters. **J. Mazuela**, T.K. Antonsson, M.J. Johansson, L. Knerr, S.P. Marsden

8:20 ORGN **24.** Catalytic asymmetric allylboration of cyclic imines for the stereodivergent synthesis of prenylated indolines and tetrahydroisoquinolines. **C. Diner**, M. Alam, S. Jonker, L. Eriksson, K. Szabo

8:40 ORGN **25.** Vic-tricarbonyl compounds in natural product synthesis: Studies in total syntheses of preussochromones. **U. Koert**, E. Kerste

9:00 ORGN **26.** Rationalization of enantioselectivity in chiral phosphoric acid-catalyzed reactions of sp^3 electrophiles using DFT calculations. **P. Champagne**, K.N. Houk

9:20 ORGN **27.** Efficient and scalable enantioselective synthesis of the axially chiral 11-β-HSD inhibitor, BMT-816336. **D.K. Leahy**, C. Chan, K. Zhu, R.L. Hanson

9:40 ORGN **28.** Enantioselective palladium-catalyzed insertion of carbene groups into N-H bonds of aromatic heterocyclesα. **D. Van Vranken**, S.C. Hiew, U. Ilandari Dewage, V. Arredondo, E. Gutman

10:00 ORGN **29.** Enantioselective photocatalytic [3+2] cylcoadditions of aryl cycloproply ketones, and strategies for developing selective photocycloadditions through dual catalysis. **E.M. Sherbrook**, T.P. Yoon, A. Amador

10:20 ORGN **30.** Enantioselective Tsuji allylation of enol acetates. **J. Liu**, S. Mishra, A. Aponick

10:40 ORGN **31.** Total synthesis of (-)-martinellic acid enabled by enantioselective copper catalyzed quinoline alkynylation. **M. Pappoppula**, F.S. Cardoso, B.O. Garrett, A. Aponick

11:00 ORGN **32.** New strategy for the first organocatalytic asymmetric γ′-selective functionalization of cyclic enones: [4+2] cycloaddition/retro-Mannich reaction. **Z. Chuncheng**, Y. Jinxing

Section E

Moscone Center
3007

Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*

O. Reiser, *Presiding*

8:00 ORGN **33.** One-pot palladium-catalysed synthesis of sulfonyl fluorides from aryl bromides. **A.T. Davies**, J. Curto, S.W. Bagley, M.C. Willis

8:20 ORGN **34.** Rhodium(III)-catalyzed C-H functionalization of 1-(2*H*)-phthalazinones at C8. **M. Huestis**

8:40 ORGN **35.** Development of new tools for the functionalization of cubane. **S.S. Bernhard**, S.L. Plunkett, M.O. Senge

9:00 ORGN **36.** Cooperative palladium and copper catalyzed hydroarylation of alkenes: A new approach to sp^2-sp^3 cross coupling. **S.D. Friis**, M.T. Pirnot, S.L. Buchwald

9:20 ORGN **37.** Solving a solved problem: The Chan-Evans-Lam amination. **A.J. Watson**

9:40 ORGN **38.** Extending the Chan-Lam coupling reaction scope via cooperative photoredox and copper catalysis. **A.J. Wommack**, J. Marshall

10:00 ORGN **39.** Development of functionalized primary alkylboronic derivatives for the Chan-Lam couplings of anilines. **T.E. Cole**, I. Han, E. Torres, G. Elliott, A. Klein

10:20 ORGN **40.** Catalytic aerobic oxidation of alcohols catalyzed by cerium complexes supported by a pentadentate Schiff-base ligand. S. Shirase, H. Tsurugi, **K. Mashima**

10:40 ORGN **41.** Double active template strategy for functional rotaxane synthesis. **J. Weiss**, J.A. Wytko, T. Hayashi, Y. Miyazaki

11:00 ORGN **42.** Visible-light mediated synthesis of aryl alkyl ketones. **S. Roslin**, L. Odell

11:20 ORGN **43.** Shining light on copper: Unique opportunities for visible-light-mediated photoredox catalysis. T. Rawner, S.K. Pagire, C. Lankes, **O. Reiser**

11:40 ORGN **44.** Temporary dearomatization as tool for a formal S_EAr on pyridines with silicon electrophiles. **S. Wübbolt**, M. Oestreich

Section F

Moscone Center
3005

New Reactions & Methodology

R. D. Broene, *Organizer*

D. A. Nagib, *Presiding*

8:00 ORGN **45.** Thermal intermolecular [3+2] cycloaddition reactions of 4-phthalimido-*N*-sulfonyltriazoles and substituted arenes. **S.M. Wilkerson-Hill**, H.M. Davies

8:20 ORGN **46.** C–H xanthylation: A synthetic platform for alkane functionalization. **W. Czaplyski**, C.G. Na, E.J. Alexanian

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

8:40 ORGN **47.** *p*-Halogenations made easy. **E. Jalali**, K. Dudley, B. Fouzia, Q. Nguyen, J. Bailey, D. Slocum

9:00 ORGN **48.** Application of alkylquinone tautomerization to the total synthesis of Calothrixin B. **L.M. Mori Quiroz**, M. Dekarske, M.D. Clift

9:20 ORGN **49.** Metal-free intermolecular aminoarylation of alkynes. **P. Rabet**, S. Boyd, M. Greaney

9:40 ORGN **50.** Para-selective halogenation and oxygenation of arenes. **S.C. Fosu**, C.M. Hambira, D.A. Nagib

10:00 ORGN **51.** Withdrawn.

10:20 ORGN **52.** Polarity-reversed carbonyl reactivity via an anomeric activation strategy. **D.A. Nagib**

10:40 ORGN **53.** Synthesis and study of 1,3-disiloxanediols with applications for hydrogen-bonding and anion-binding catalysis. **K. Diemoz**, A. Kelly, A.K. Franz

11:00 ORGN **54.** New strategies for aromatic substitution; the development of S_NAr catalysis. **J.D. Weaver**, S. Senaweera

11:20 ORGN **55.** Broad spectrum enolate equivalent for catalytic chemo-, diastereo-, and enantioselective addition to N-boc imines. **C. Hung**, B.M. Trost

11:40 ORGN **56.** Glycerol: A C3 bio-based platform chemical for alternative technologies. **C. Len**

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

SUNDAY AFTERNOON

Section A

Moscone Center

3018/3022

Herbert C. Brown Award for Creative Research in Synthetic Methods: Symposium in honor of Bruce H. Lipshutz

Financially supported by Aldrich (Millipore Sigma), ACS Green Chemistry Institute

D. M. Huryn, *Organizer, Presiding*

1:10 Introductory Remarks.

1:15 ORGN **57.** Ligand-accelerated C–H activation: From fundamentals to applications. **J. Yu**

1:55 ORGN **58.** New enzymes for green chemistry. **F.H. Arnold**

2:35 ORGN **59.** Photoredox/nickel dual catalytic cross-coupling and related processes. **G.A. Molander**

3:15 ORGN **60.** Understanding the reduction mechanism Pd(II) to $L_nPd(0)$ (n = 1 and 2) catalysts for organic synthesis. **T. Colacot**

3:55 Introduction of Awardee.

4:00 ORGN **61. Award Address** (Herbert C. Brown Award for Creative Research in Synthetic Methods sponsored by the Purdue Borane Research Fund & the Herbert C. Brown Award Endowment). Betting on nature: Making the switch to environmentally responsible synthetic organic chemistry in water. **B.H. Lipshutz**

Section C

Moscone Center

3011

Biologically-Related Molecules & Processes

R. D. Broene, *Organizer*

A. R. Narayan, *Presiding*

1:30 ORGN **62.** High-throughput evaluation of small-molecule catalyst libraries: Development of an amphiphilic, DNA-encoded reaction discovery platform. **K.D. Hook**, R. Hili

1:50 ORGN **63.** Rearrangement chemistry of aryl and heteroaryl sulfonamides. **W. Martin**, R.D. Bowen, R. Gallagher, A. Saidykhan

2:10 ORGN **64.** Molecular approaches to photocontrol of biological singlet dioxygen. **Y. You**

2:30 ORGN **65.** Selective functionalisation and diversification of halogenated compounds through mild aqueous cross-coupling methodologies: From organic molecules to natural products. **C. Pubill-Ulldemolins**, M. J. Corr, S. V. Sharma, E. Marelli, R. Goss

2:50 ORGN **66.** Exploration of advance synthetic processes for generating heterocyclic scaffolds: Synthetic scope and mechanistic insight. **S. Sharma**, D.M. Sawant, R.T. Pardasani

3:10 ORGN **67.** Progress towards an anti-inflammatory based on the aurone scaffold. **Z.E. Taylor**, J.K. Noe, G. Flowers, H. Park, A.L. Farone, S.T. Handy

3:30 ORGN **68.** Pd-catalyzed arylation of cyclic and spirocyclic diamines under aerobic conditions. **S.W. Reilly**, R.H. Mach

3:50 ORGN **69.** Construction of a new eighteen-membered core structure for simplified and stabilized zampanolide mimics. **Q. Chen**, R. Wang, G. Chen, X. Zhang

4:10 ORGN **70.** Privileged diversity oriented organic synthesis: Modular one-step route for the synthesis of novel compound collections for phynotypic screening. **T.H. Altel**, R. Ralph Mazitschek

4:30 ORGN **71.** Leveraging biosynthetic enzymes for complex molecule synthesis. **A.R. Narayan**

Section D

Moscone Center

3009

Asymmetric Reactions & Syntheses

R. D. Broene, *Organizer*

M. Harmata, *Presiding*

1:00 ORGN **72.** New catalytic, asymmetric (4+3)-cycloaddition reaction. M. Topinka, K. Zawatzky, C.J. Welch, **M. Harmata**

1:20 ORGN **73.** Asymmetric synthesis of Rauhut-Currier type products by a regioselective Mukaiyama reaction under bifunctional catalysis. **M. Frías Rodríguez**, R. Mas-Balleste, S. Arias, C. Alvarado, J.J. Alemán

1:40 ORGN **74.** Enantioselective allylic C–H oxidation of terminal olefins to isochromans by palladium(II)/chiral sulfoxide catalysis. **W. Liu**, S.E. Ammann, M. White

2:00 ORGN **75.** Ligand-accelerated enantioselective methylene C(sp^3)–H bond activation. **G. Chen**

2:20 ORGN **76.** Global collaborations in asymmetric synthesis to catalyze discovery and development. **M. Chorghade**

3:00 ORGN **77.** Process development for β2 adrenergic receptor agonist moiety via ruthenium-catalyzed asymmetric reduction. **M. Komiyama**, T. Itoh, Y. Sato, M. Tabe

3:20 ORGN **78.** Highly efficient and enantioselective synthesis of deoxypropionates and isoprenoids. **M. Komiyama**, S. Xu, H. Li, E. Negishi

3:40 ORGN **79.** Chiral dinuclear rhodium(III) complexes as catalyst precursors for asymmetric hydrogenation of simple olefins. K. Higashihara, K. Higashida, H. Nagae, **K. Mashima**

4:00 ORGN **80.** Brønsted-acids in template mediated asymmetric synthesis: Mechanistic understanding of azomethine imine cycloaddition reactions. **H. Subramanian**, M.P. Sibi

Section E

Moscone Center

3007

Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*

T. W. Funk, *Presiding*

1:00 ORGN **81.** Ruthenium(II)-catalyzed C-H activation. **L. Ackermann**

1:20 ORGN **82.** Ruthenium catalyzed ortho-C–H halogenation: Switching the chemoselectivity of iodine monochloride by catalyst choice. **D. Bunting**, C.J. Teskey, M. Greaney

1:40 ORGN **83.** Development of heterogeneous and homogeneous catalysts for directed C-H halogenation reactions: Implications in late stage functionalization. **M.J. Johansson**, B. Martin-Matute, X. Zou, E. Erbing, V. Pascanu, F. Carson, J. Malmberg, A. Sanz-Marco, A. Vázquez-Romero, J. Su

2:00 ORGN **84.** Development of a highly diastereoselective α-arylation of cyclobutyl nitriles. **M.E. Dalziel**, P. Chen, D.E. Carrera, H. Zhang, F. Gosselin

2:20 ORGN **85.** Synthesis of indolines by enantioselective C–H insertion reactions of donor-donor metal carbenoids. **R. Squitieri**, C.N. Penrod, J.T. Shaw

2:40 ORGN **86.** Sustainable approaches to C–H functionalization processes. F. Ferlin, S. Santoro, L. Ackermann, **L. Vaccaro**

3:00 ORGN **87.** Rhodium-catalyzed enantioselective silylation of aryl C–H bonds: Synthetic and mechanistic studies. **T. Lee**, J.F. Hartwig

3:20 ORGN **88.** Multicomponent coupling reactions on a zirconocene template. **J. Stec**, R.J. Whitby

3:40 ORGN **89.** Palladium-catalyzed processes involving olefin insertion, enolate coupling and radical alkylation. **J. Zhou**

4:00 ORGN **90.** Gold-catalyzed domino aminative homodimerization of *ortho*-alkynylbenzaldehydes providing tetracyclic 1,2-dihydronaphthalene derivatives. **A. Ruch**, L.M. Slaughter, F. Kong, V. Nesterov

4:20 ORGN **91.** Reaction kinetics of (3,4-diphenylcyclopentadienone)iron carbonyl-catalyzed alcohol oxidations and carbonyl reductions. **T.W. Funk**

Section F

Moscone Center

3005

New Reactions & Methodology

R. D. Broene, *Organizer*

H. A. Lindsay, *Presiding*

1:00 ORGN **92.** Modular cuI-proline catalyzed one-pot route for the rapid access of privileged small and medium ring systems. **T.H. Altel**, V. Srinivasulu

1:20 ORGN **93.** Orthogonal dual-click diyne for CuAAC and/or SPAAC couplings. **R.R. Ramsubhag**, G.B. Dudley

1:40 ORGN **94.** Ligand-controlled silylation and reduction of aryl ammonium salts using nickel *N*-heterocyclic carbene catalysis. **A.W. Rand**, J. Montgomery

2:00 ORGN **95.** Development of an interrupted carbonyl-olefin metathesis reaction. **R. Watson**, J. Ludwig, D. Nasrallah, J. Gianino, C. Schindler

2:20 ORGN **96.** Halotrimethylsilane-nitrate salts: An efficient reagent system for versatile synthetic applications. **T. Mathew**, S. Roshandel, L. Gurung, G. Prakash, G. Olah

2:40 ORGN **97.** One step beyond: Diversifying cycloisomerization products through new reactions. A. Pathak, **M.W. Peczuh**, J. Saha

3:00 ORGN **98.** Solvent compatibility with acridinium labels: Cyrene evaluation. **J. Grote**

3:20 ORGN **99.** Diazepane carboxylates as organocatalysts: The first organocatalytic Cope rearrangement and application to the Diels-Alder and polyene cyclizations. **J. Gleason**, D. Kaldre, N. Haggman, F. Larnaud, S. Plamondon

3:40 ORGN **100.** Microwave-promoted iminyl radical fragmentations: A practical and efficient method of functionalization. **M. Jackman**, S. Im, S.R. Bohman, A.L. Garrity, S.L. Castle

4:00 ORGN **101.** Piperidines via a microwave-assisted aza-Prins reaction. **H.A. Lindsay**, A. Green, A. Havens

4:20 ORGN **102.** Research progress on interrupted pummerer cyclization. **X. Li**, R.G. Carter

4:40 ORGN **103.** One-pot tandem Diels-Alder/Nazarov cyclization to generate advanced tricyclic intermediates. **R.A. Carmichael**, P. Sophanpanichkul, W. Chalifoux

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

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LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

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SUNDAY EVENING

Section A

Moscone Center
West Hall

Asymmetric Reactions & Syntheses

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **104.** Phosphothreonine as a catalytic residue in peptide-catalyzed asymmetric transfer hydrogenations. **C.R. Shugrue**, R.M. Lackner, S.J. Miller

ORGN **105.** Synthesis of polypropionate building blocks for complex natural products. **D. Galler**, M. Calder

ORGN **106.** Camphor-derived 1,3-diamine bifunctional organocatalysts. **S. Ricko**, J. Svete, B. Štefane, U. Grošelj

ORGN **107.** Synthesis and DNA binding studies of azinomycin chromophore analogues. **S. Pacheco**, A. Nazarian

ORGN **108.** Asymmetric organocatalytic Michael additions of methyl thioglycolate to various acceptors. **D. Tözendemir**, C. Tanyeli

ORGN **109.** Bioinspired organocatalytic decarboxylative aldol reaction of aldehydes and ketones: Formal synthesis of chiral fluralaner. **J. Sim**, H. Bae, C. Song

ORGN **110.** Benzylisobornyl derivatives as chiral auxiliaries and chiral organocatalysts. **M.K. Kennedy**, **P.J. Hartfield**, **A.J. Dahl**, **D.E. Lewis**

ORGN **111.** Synthesis of aldehyde substrates for an organocatalyzed enantioselective β-alkylation reaction. **M.E. Akana**, S. Konda, J.C. Zhao

ORGN **112.** Separate ways: Efforts to resolve planar chiral [13]-macrodilactones. **J. Lawrence**, M.W. Peczuh

ORGN **113.** Transition state analogues as mechanistic probes for asymmetric desymmetrization by cinchona alkaloid-based catalysts. **E. Emmings**, G.E. Hofmeister, D.G. Alberg

ORGN **114.** Synthesis and characterization of fluorinated curcumin-pyrazoline derivatives. **C. Kannigadu**, N. Koorbanally

ORGN **115.** Enantioselective synthesis indenes via chiral Brønsted acid catalyzed Nazarov-type cyclization of β-amino-1,4-enynols. **J. Jin**, Y. Zhao, P.W. Chan

ORGN **116.** Chemo- and stereodivergent synthesis of piperidine derivatives catalyzed by modularly designed organocatalysts. N.K. Rana, **J.C. Zhao**

ORGN **117.** New quinine-based squaramide catalyst and its evaluation in the asymmetric aza-Friedel-Crafts reactions of isatin-derived ketimines. **S. Karahan**

ORGN **118.** Regio-, diastereo-, and enantioselective borylative dearomatization of indoles using copper(I) catalysis. **K. Hayama**, K. Kubota, H. Iwamoto, H. Ito

ORGN **119.** Enantioselecitve organocatalytic synthesis of cyclohexenone and 4*H*-pyran derivatives: A divergent approach. **X. Ding**, N. Heberer, B. Borhan

ORGN **120.** Synthesis and application of amino-acid condensed δ-lactams. **I. Jahan**, M.E. Taylor, G.A. Kraus, A.E. Russell, M.O. Abdalla

ORGN **121.** Asymmetric synthesis of γ-lactones and related chiral building blocks through reaction of enediolates with vinyl onium salts. **S. Kaster**, N. Peraino, N. Kerrigan

ORGN **122.** Synthesis of 1,2,4-dioxazinanes via aza-Michael desymmetrization. **T.R. Vavrek**, R. Marfatia, M. Abdel, H. Sharma, J. Fedor, **D.M. Rubush**

ORGN **123.** Enantioselective oxyallyl cation catalysis: A theoretical study. **C. He**, K.N. Houk

ORGN **124.** Organic/metallic catalytic system for the asymmetric reactions of disubstituted ketenes. **D. Paull**, E. Barth

ORGN **125.** Enantioselective organocatalysis: Synthesis and NMR studies of transition state analogues. **C. Leahy**, D.G. Alberg, G.E. Hofmeister

ORGN **126.** Effect of acid concentration on the dynamic kinetic resolution in the cyclocondensation synthesis of ß-alkyl-5,5-bicyclic lactams. P.T. Buonora, **D. Nguyen**

ORGN **127.** Working with challenging substrates in catalytic enantioselective reactions: Understanding cooperative modes of activation in template-based catalytic reactions. **H. Subramanian**, M.P. Sibi

ORGN **128.** Synthesis of bivalent organothiophosphates and their inhibition of butyrylcholinesterase: A potential therapeutic for Alzheimer's disease. **A. Tahira**

ORGN **129.** Development and tandem EPR study of an asymmetric Cu(II)-catalyzed spiroannulation. **B. Armstrong**, R.I. Sayler, B. Shupe, J.P. MacDonald, R. Britt, A.K. Franz

ORGN **130.** Withdrawn.

ORGN **131.** Enantioselective Friedel-Crafts reaction of indoles and pyrroles using a cation-binding catalyst. **M. Kim**, L. Xue, Y. Liu, S. Paladhi, S. Park, H. Yan, C. Song

Section B

Moscone Center
West Hall

New Reactions & Methodology

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **132.** Chiral diaziridines for the synthesis of five-membered ring nitrogen-containing heterocycles. **J. Lizza**, G. Moura-Letts

ORGN **133.** Withdrawn.

ORGN **134.** Synthesis of (Z)-2-((tert-butyldimethylsilyl)oxy)-3-(phenylthio) acrylaldehyde. **M. Topinka**, M. Harmata

ORGN **135.** (4+3)-Cycloaddition reactions of oxidopyridinium species. **C. Fu**, N. Lora, P.L. Kirchhoefer, D.R. Lee, E. Altenhofer, C. Barnes, M. Harmata

ORGN **136.** Investigation of transannular epoxide-opening toward bioactive pyrrolizidine alkaloids. **C. Williams**, **B. Schafer**, B. Wesley, A. Kaplan, E.E. Cleary, K.E. Allen, A. Betrus, M.M. Majireck

ORGN **137.** Synthesis of *N*-(1-alkoxyvinyl) pyridinium salts and preliminary investigation of their utility in organic synthesis. **J. Shapiro**, J. Sonberg, H. Ferris, C. Williams, C. Kriley, E.W. Reinheimer, M.M. Majireck

ORGN **138.** Preparation, structure and reactivity of pseudocyclic benziodoxole tosylate reagents. **M. Shea**, **M. Liebl**, S. Klasen, K. Nguyen, G. Rohde, **A. Yoshimura**, A. Saito, V. Nemykin, V.V. Zhdankin

ORGN **139.** Metal-free imination of sulfides using tosyliminoiodane reagent. **C. Makitalo**, **J. Fuchs**, **A. Yoshimura**, A. Saito, V.V. Zhdankin

ORGN **140.** Assigning the absolute configuration of amines using the competing enantioselective conversion method. **A. Burtea**

ORGN **141.** Stereospecific nickel-catalyzed cross-coupling reactions of benzylic ethers: Investigation of ring-opening reactions and active catalyst identity. **D. Dawson**, E.R. Jarvo, E. Tollefson, C. Osborne

ORGN **142.** Withdrawn.

ORGN **143.** ipso-Bromination/iodination of arylboronic acids: Application of poly(4-vinylpyridine)-bromine/iodine complex as efficient reagent. **F. Fu**, L. Gurung, M. Czaun, T. Mathew, S.G. Prakash, G. Olah

ORGN **144.** Halogenation and ipso-nitration of cinnamic acids: Halotrimethylsilane-nitrate, an efficient reagent system. **S. Roshandel**, L. Gurung, T. Mathew, G. Prakash, G. Olah

ORGN **145.** Four-fold alkyne benzannulation to afford chiral peropyrenes. **K.M. Magiera**, W. Yang, W. Chalifoux

ORGN **146.** Efficient synthesis of bicylco[4.4.0]decanes by tandem Diels-Alder of activated alkynes. **J.A. Horton**, A.M. O'Loughlin, W. Chalifoux

ORGN **147.** Tandem diels-alder/Nazarov cyclization of ß-silyl-substituted aryl ynones. R.A. Carmichael, **P. Sophanpanichkul**, W. Chalifoux

ORGN **148.** Studies towards the iron(II)-promoted stereoselective haloamination of alkenes. N. Chang, B. Selover, L. Mir, **G. Moura-Letts**

ORGN **149.** Intramolecular dipolar cycloadditions of enediaziridines. **G. Haun**, D. Almond, G. Moura-Letts

ORGN **150.** Potassium phosphate-catalyzed one-pot synthesis of 3-aryl-2-oxazolidiones from epoxides, amines, and atmospheric carbon dioxide. **Y.K. Chung**, U. Seo

ORGN **151.** Organocatalytic activation of isocyanides: N-heterocyclic carbene-catalyzed enaminone synthesis. **J. Kim**, S. Hong

ORGN **152.** Development of CLAmP: Rational design of a carbonyl dication synthon that facilitates the one-pot synthesis of unsymmetrical ketones. **S. Heller**, J.N. Newton, T. Fu, R. Sarpong

ORGN **153.** Transition-metal-free regioselective alkylation of heterocyclic *N*-oxides using 1,1-diborylalkanes as alkylating reagents. **S. Cho**

ORGN **154.** Selective α-oxo C(sp^3)-H thioesterification of ether. **B. Kang**, S. Hong

ORGN **155.** Photoredox/nickel dual-catalysis-enabled cross-coupling of sulfonamides and aryl halides. **T. Kim**, E.B. Corcoran, D.W. MacMillan

ORGN **156.** Improved synthesis of lamivudine and emtricitabine. **D. Mandala**

ORGN **157.** Withdrawn.

ORGN **158.** Formylthioester: Highly chemoselective formylating reagent in palladium-catalyzed cross-coupling reaction of organozincs. R. Haraguchi, **S. Tanazawa**, S. Fukuzawa

ORGN **159.** Novel, sustainable catalyst activation: Electrochemical reduction of titanocene dichloride and applications. **T. Olyschlaeger**, A. Gansäuer

ORGN **160.** Selective monooxidation of symmetric dialdehydes in aqueous solvent. P. Kattanguru, R. Ogawa, **S. Niwayama**

ORGN **161.** Biocatalytic reduction of ketones and imines using *Daucus carota root*. **A. Bogetti**, R. Kroeker Sachs

ORGN **162.** Trichloroisocyanuric Acid (TCCA) as a reagent for chlorolactonization and chlorocyclization. S. Jana, **I. Hackett**, V. Dragojlovic

ORGN **163.** Regioselective construction of N^2-acyl-C^4-aryl-aminoimidazoles. **E. Kirkeby**, J. Salvant, K. Guillen, R. Looper

ORGN **164.** Epoxide approach towards the synthesis of (-)-dolabriferol and (-)-dolabriferol B. **K. Morales**, J.A. Prieto

ORGN **165.** Palladium catalyzed homo coupling reactions with in situ formed organolithium reagents, and its application in the total synthesis of Mastigophorene A. **D. Heijnen**, J. Buter, V. Hornillos, C. Vila, A. Minnaard, B. Feringa

ORGN **166.** Formal [2+2+2] photoredox synthesis of naphthalene derivatives using aniline as traceless directing group. **Q. Wang**, N. Zheng

ORGN **167.** Construction of an azasteroid library. **M. Charaschanya**, J. Aube

ORGN **168.** Reductive ketyl radical cyclizations towards the total synthesis of the plakortone family of natural products. **N. Foy**, J. Cannon

ORGN **169.** Development of an auxiliary-directed enolate alkylation for unnatural amino acid synthesis. **N. Dwulet**, J. Cannon

ORGN **170.** Pd-catalyzed difunctionalization of unactivated olefins by tandem Heck coupling/enolate cyclization. **R.K. Dhungana**, B. Shrestha, R. Thapa Magar, R. Giri

ORGN **171.** Tetraphenylphosphonium tetrafluoroborate/1,1,1,3,3,3-hexafluoroisopropanol (Ph_4PBF_4/HFIP) effecting epoxide-initiated cation–olefin polycyclizations. **Y. Tian**, J. Qu

ORGN **172.** Halogen bonding induced Friedel-Craft-type alkylation of thiophenes with α,β-unsaturated carbonyl compounds. **Y. Ge**, W. He, C. Tan

ORGN **173.** Arenophile-mediated dearomative reductions. **M. Okumura**, S.M. Nakamata Huynh, J. Pospech, D. Sarlah

ORGN **174.** Anodic coupling of imine with nitrile: Transition-metal-free synthesis of quinazoline derivatives. H. Hung, **Y. Huang**

ORGN **175.** Experimental methodology of C-amination at the C-4 position of triacetic acid lactone. **M.E. Taylor**, G.A. Kraus, U.K. Wanninayake, Y. Qu

ORGN **176.** Dehydrogenative N-formylation and N-methylation of amines catalyzed by ruthenium pincer complex. **G. Choi**, S. Kim, S. Hong

ORGN **177.** Investigation of the Lewis-base catalyzed $TMSCF_3$ additions to 2-halogenated carbonyls. **N. Heth**, **S. Rouleau**, T.A. Davis

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ORGN **178.** Palladium catalyzed electrophilic fluorination of aryl oxazolines via C-H activation. **D. Gutierrez**

ORGN **179.** Synthesis of hemilabile *N,P* ligands with one, two or three chiral centers. **J. Kukowski**, I.P. Smoliakova

ORGN **180.** New approaches to the chemical synthesis of ketones from organoboranes by using chlorochromate reagent. E.J. Parish, G. Ren, Y. Lo, **H. Honda**, **M. Hsiao**, T. Wei

ORGN **181.** Exploring the photochemistry of carbonyl-decorated carbenes: N,N'–diamidocarbenes (DACs). **T.A. Perera**, T.W. Hudnall

ORGN **182.** Novel application of new synthetic reagents for the oxidation of activated methylene groups for allylic oxidation. **G. Ren**, E.J. Parish, Y. Lo, **H. Honda**

ORGN **183.** Lewis acid catalyzed 1,4-addition of nucleophiles to α, β-unsaturated ketones. **T.J. Rauwolf**, R.S. Mohan

ORGN **184.** Metal-free synthesis of 1,3-disiloxanediols and methods toward chiral variants for asymmetric catalysis. **A. Kelly**

ORGN **185.** One-pot tandem oxidative dearomatization/[4+3] cycloaddition: Masked o-benzoquinone with diaza-oxyallyl cation. **K. Lee**, H. Hsieh

ORGN **186.** Novel counterion for soluble anhydrous fluoride. B. Wang, **E. Linstad**, H. Sun, S.G. DiMagno

ORGN **187.** Synthesis of annulated α-carbolines via metal-catalyzed cyclizations involving cyanamides. **S. Wrenn**, S.P. Mulcahy

ORGN **188.** Practical stereocontrolled synthesis of vicinal halohydrins and haloamines from vinyl epoxides and vinyl aziridines. **L. Weselinski**, M.J. Grillo, M. Tanasova

ORGN **189.** Development of new synthetic methodologies utilizing the decomposition products of alkyl triazabutadienes. **D. Knyazeva**, J.C. Jewett

ORGN **190.** Modifications and mechanistic determination of the Ley-Griffith oxidation of alcohols. **P.W. Moore**, Y. Jiao, T. Zerk, C. Read, P. Mirzayans, L. Ng Qi Sheng, J. Hooker, P. Bernhardt, C. Williams

ORGN **191.** Mechanistic insight into the synthesis of β-lactones via isothiourea-catalysed enantioselective formal [2+2] cycloaddition. **D. Barrios Antúnez**, A.D. Smith

ORGN **192.** Green protocol for the preparation of silyl enol ethers and their application in the synthesis of fine chemicals. **D. Lanari**, M. Curini, C. Morozzi

ORGN **193.** Five-membered ring closure via intramolecular nucleophilic attack by nitrogen ylides on C=C bond of cyclopropenes. **C. Barrett**, M.A. Rubin

ORGN **194.** Why LogD matters to the synthetic organic chemist: How lipophilicity and pKa interact to affect success or failure in acid-base separations of amine mixtures. **D.J. O'Mahony**, R.J. Johnson, C. Francavilla

ORGN **195.** Studies on the alkylation of phenolate in an organofluorine solvent. **M. Kim**, M. Ryu, Y. Son, Y. Choi, J. Jung

ORGN **196.** Synthesis and reactivity of trifluoromethyl iodonium salts: Mechanistic and synthetic significance. **A.V. Samant**, J.N. Brantley, D. Toste

ORGN **197.** New microwave-promoted transformation of iminyl radicals. **S. Im**, M. Jackman, S.R. Bohman, A.L. Garrity, S.L. Castle

ORGN **198.** Tailoring a chalcone synthesis for use with deuterated starting materials. **C.A. Gehman**, C. Hamann

ORGN **199.** Discovery of a novel synthetic method to form binaphthyltetraone compounds. **V. Jha**, C. Stevens, E. Stevens, J. Sridhar

ORGN **200.** New strategy for the preparation of 3, 4-hydroxypyridinone (HOPO) siderophores using selective N-alkylation of 3-benzyloxy-2-methyl-4-pyridinone. **D. Favela**, A.S. Gopalan, H.K. Jacobs

ORGN **201.** Exploration of dihydrofuro-isoxazolines based on Intramolecular Silyl Nitronate Cycloadditions (ISNC) as branch points for novel isoxazoline compounds. J.L. Duffy-Matzner, **K.G. Stevens**

ORGN **202.** Post-synthetic modification of drug candidates via C-H functionalization. **S.C. Fosu**, C.M. Hambira, D.A. Nagib, J. Fuchs

ORGN **203.** Polarity-reversed radical cascade for the functionalization of heteroarenes. **J. Lear**, D.A. Nagib

ORGN **204.** Nucleophilic, radical, and electrophilic trifluoromethylation reagents from fluoroform. **J.B. Geri**, N.K. Szymczak

ORGN **205.** Simple, stereospecific method for inversion of alcohols. **C. Paquin**, D.W. Boerth

ORGN **206.** Developing a path to chiral aziridines through asymmetric copper hydride reduction. **R. Turro**, J. Unger

ORGN **207.** Direct, regioselective *N*-alkylation of 1,3-azoles. **R. Graceffa**

ORGN **208.** Triiodide-mediated δ C-H amination of amines and alcohols. **E. Wappes**, K. Nakafuku, S.C. Fosu, D.A. Nagib

ORGN **209.** Transition-metal-free decarboxylative amidation and their intramolecular cyclization for the synthesis of N-heteocycles and its application to the preparation of marketed drug, sildenafil. **K.V. Patel**, K. Tummalapalli, N. Dayal, J. Laha

ORGN **210.** Alkylation of heterocycles through a photoredox catalytic reductive decarboxylation. **E.J. McClain**, A. Sun, J.W. Beatty, C. Stephenson

ORGN **211.** Unusual ring-expansion reaction to prepare 9-Nitro-5H-spiro[benzo[b]tetrazolo[1,5-d] oxazepine-4,2'-oxirane]. **R.S. Kolluri**

ORGN **212.** Redox-active esters in Ni-catalyzed cross-coupling reactions. **J.T. Edwards**, J. Cornella, T. Qin, J. Wang, R. Merchant, K.S. McClymont, K.W. Knouse, C. Li, L. Malins, S. Kawamura, C. Pan, L. Wimmer, T. Chen, a. Novak, J.Z. Zhong, R. Mills, R. Gianatassio, M. Schmidt, C. Yuan, B. Maxwell, B. Vokits, S.A. Shaw, M.D. Eastgate, P.S. Baran

ORGN **213.** Alkaloid-like substructures via photoredox catalysis: Synthesis of 1-aminonorbornanes. **T.M. Sodano**, D. Staveness, C. Stephenson

ORGN **214.** Regioselective benzosultam formation via silver-catalyzed nitrene insertion. **B. Sheffer**, R.J. Scamp, J.M. Schomaker

ORGN **215.** Lewis and Brønsted acid-catalyzed allylsilane oligomerization. **B. Wigman**, A.K. Franz, B. Armstrong

ORGN **216.** Synthetic utility of boracarboxylated styrene derivatives. **T. Perrone**, T.W. Butcher, S. Knowlden, E.J. McClain, B.V. Popp

ORGN **217.** Lanthanum(III)-catalyzed three-component reaction of coumarin-3-carboxylates for the synthesis of indolylmalonamides and analysis of their photophysical properties. **J. Jennings**, C.P. Bhatt, B.I. Gomez, A. Nguyen, A.K. Franz

ORGN **218.** 3-Methylene-2,4-chromandione *in situ* trapping. **F. Popowycz**, M. Boulven, A. Montagut-Romans

ORGN **219.** Synthesis of nitro, amino, nitro/OR, and amino/OR substituted distyrylbenzene and polyphenylene vinylene. **A.I. Torres Burgueno**

ORGN **220.** Development of new methodologies for GSK medicinal chemistry projects. **E. Talbot**, R. Griffiths, J. Spencer, R.P. Law, S. Ukuser, C. Jamieson, G.A. Burley

Section C

Moscone Center
West Hall

Metal-Mediated Reactions & Syntheses

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **221.** Improvement in cross-coupling reactions by heterobimetallic nickel catalysis. **H. Nazari**

ORGN **222.** Nickel-catalyzed asymmetric reductive cross-couplings with vinyl bromide electrophiles. **J. Hofstra**, N. Suzuki, K. Poremba, S.E. Reisman

ORGN **223.** Nickel-catalyzed direct arylation of oxazoles: Benchmarking the influence of electronic, steric and leaving group variations in the phenolic electrophiles. **D. Steinberg**, **M.C. Turk**, D. Kalyani

ORGN **224.** Nickel-catalyzed cross-coupling of aromatic nitriles and azoles. **M.G. Hanson**, N. Olson, **G. Wilson**, D. Kalyani

ORGN **225.** Optimization of a palladium-catalyzed C-N coupling towards the robust synthesis of a RORc ligand. **D. Lao**, L.E. Sirois, R. Angelaud, J. Xu, F. Gosselin

ORGN **226.** Palladium-catalyzed ortho-arylation of benzamides using a removable directing group. **Y. Shen**, W. Lee, D.A. Gutierrez, J.J. Li

ORGN **227.** Palladium catalyzed direct arylation of nitroarenes using tosylates and mesylates. **Y. Aschenaki**, A. Schnaith, S. Davick, Z. Yi, R. Wander, R. Daley, D. Kalyani

ORGN **228.** Palladium-catalyzed reactions of fluoroalkenes. **R. Thornbury**, D. Toste

ORGN **229.** Pd mediated selective functionalisation and diversification of biologically relevant halogenated molecules through mild cross-coupling methodologies in water. **C. Pubill-Ulldemolins**, S. V. Sharma, M. J. Corr, E. Marelli, R. Goss

ORGN **230.** Pd^{2+} detection in water-based Suzuki-Miyaura coupling reaction using colorimetry with squaraine dyes. **K. Novosad**, D. Janzen, R.S. Majerle

ORGN **231.** Transmetalation of alkylzirconocenes: Copper-catalyzed alkyl–alkynyl cross-coupling with bromoalkynes. **K. Indukuri**, O. Riant

ORGN **232.** Late stage copper-mediated fluorination with PET imaging applications. **K.J. Makaravage**, A.F. Brooks, A. Mossine, M.S. Sanford, P.J. Scott

ORGN **233.** Activation of disilanes with copper(I)-alkoxides. **R. Van Hoveln**, B. McCarty, B. Thomas

ORGN **234.** Application of copper(I) bisphenanthroline complexes in enantioselective photoredox reactions. **M.R. Jilek**, M.R. Hurst, S.A. Souder, **K.H. Jensen**

ORGN **235.** Copper-catalyzed synthesis of iminoquinolizines and aminoindolizines. **A.K. Isaacs**, **B. Ghiano**, T. Correia

ORGN **236.** Stereoselective borylative radical cyclization with copper(I) catalyst. **H. Iwamoto**, S. Akiyama, K. Hayama, H. Ito

ORGN **237.** Copper-mediated C–H chlorination by trichloroacetamide using a directing group. **W. Lee**, Y. Shen, D.A. Gutierrez, J.J. Li

ORGN **238.** Highly diastereoselective (*Z,*)-5-trimethylgermyl-2-alkenones via organoboranes. **N.G. Bhat**

ORGN **239.** New diastereoselective synthesis of (Z)-trisubstituted alkenes containing allyl and biphenyl moieties *via* organoboranes. **N.G. Bhat**

ORGN **240.** Highly diastereoselective (*Z, Z)*-ditrimethylgermyl substituted dienes via organoboranes. **N.G. Bhat**

ORGN **241.** New diastereoselective synthesis of (*Z)*-trisubstituted alkenes containing a cyclohexyl and biphenyl moieties via organoboranes. **N.G. Bhat**

ORGN **242.** Synthesis of novel, air- and moisture-stable tris(trimethylsilyl)silylborane reagents for boryl substitution and silaboration reaction. **R. Shishido**, E. Yamamoto, H. Ito

ORGN **243.** Rhodium-catalyzed addition–cyclization–rearrangement cascade of alkynylhydrazones. **K. Choi**, H. Park, C. Lee

ORGN **244.** Development of rhodium catalyzed carbon-carbon bond formation to thiochromones and N-analogues. **F. Guo**, B. Graves, J. Malcolm, S. Graham

ORGN **245.** Development of Fischer-type carbene-based ruthenium olefin metathesis catalysts. **K. Song**, K. Kim, S. Hong

ORGN **246.** Controlled monoisomerization of 1-alkenes mediated by a 16-electron ruthenium catalyst. **E.R. Paulson**, C.E. Moore, A.L. Rheingold, D.B. Grotjahn

ORGN **247.** Reductive elimination from Au(III). **M. Levin**, D. Toste

ORGN **248.** Enantioselective Au(III) catalysis. **P. Bohan**, D. Toste

ORGN **249.** Synthesis of novel NHC-Au(I) complexes with extremely bulky groups. **R. Ma**, T. Seto, B.W. Gung

ORGN **250.** Gold and Brønsted acid-catalyzed cycloisomerization of 1,8-diynyl vinyl acetates to bicyclo[2.2.1]hept-2-en-7-ones. **X. Chen**, D.P. Day, W. Teo, P.W. Chan

ORGN **251.** Synthesis of β-carbolines via a silver-mediated oxidation of tetrahydro-β-carbolines. **B. Sierra**, S. Durham, J. Tran, M. Gomez, S.C. Eagon

ORGN **252.** Silver catalyzed 1,3-acyloxy migration/diels-alder reaction of 1,4,9-dienyne esters to partially hydrogenated isoquinolines. **Y. Zhao**, **J. Jin**, **J. Boyle**, **B. Lee**, **P.W. Chan**

ORGN **253.** Transformation of amides into highly functionalized triazolines *via* Mo(CO)6 catalyzed reduction. **T. Slagbrand**, A. Volkov, M.P. Trillo, G. Tinnis, H. Adolfsson

ORGN **254.** Towards novel cobalt catalyzed C-H activation strategies. **k. suppan**

ORGN **255.** Enantioselective additions of allyl indum reagents to aldehydes. **A. Beckemeyer**

ORGN **256.** Novel route to arylated fluoroalkyl bromide building blocks through α-bromo-ω-silyl disubstituted perfluoroalkanes. **P.T. Kaplan**, D.A. Vicic

ORGN **257.** Mechanistic aspects of fluorination reactions with fuoro-benziodoxol reagent. **N. Ilchenko**, M. Hedberg, B.O. Tasch, K.J. Szabo

ORGN **258.** Substrate scope study of tandem acyl C–O/aryl C–H bond activation. **P. Gemmel**, C. Anderson, N. Serratore, S.J. Underwood, C.J. Douglas

ORGN **259.** Lewis acid-mediated, microwave-assisted cycloaddition of allylsilanes with donor-acceptor cyclopropanes. **M. Smith**, E. Finney

ORGN **260.** Withdrawn.

ORGN **261.** Ru-catalyzed selective imine formation from nitriles and secondary alcohols through hydrogen-transfer strategy. **D. Kim**, B. Kang, S. Hong

ORGN **262.** Novel application to the allylic oxidation of steroids with pyridinium dichromate and pyridinium chlorochromate. **Y. Lo**, G. Ren, E.J. Parish, **H. Honda**, T. Wei

ORGN **263.** Effects of the anion X in Cp_2TiX-catalyzed reactions. **R. Richrath**, A. Gansäuer

ORGN **264.** Nitrosoarenes as building blocks for nitrogen-functionalized arenes. **A. van der Werf**, M. Hribersek, N. Selander

ORGN **265.** Highly active titanocene catalysts for epoxide hydrosilylation: Synthesis, theory, kinetics, EPR spectroscopy. **S. Klare**, D. Schwarz G. Henriques, K. Zimmer, A. Meyer, E. Rojo-Wiechel, M. Bauer, R. Sure, S. Grimme, O. Schiemann, R.A. Flowers, A. Gansäuer

ORGN **266.** Transannular Pauson-Khand cyclization reactions of macrocyclic dicobalt hexacarbonyl-alkyne complexes. B. Boon, S. Karabiyikoglu, **C.A. Merlic**

ORGN **267.** Directing group assisted remote meta C–H bond functionalization. **A. Maji**, D. Maiti

ORGN **268.** Titanium-mediated synthesis of substituted cyclobutanes. J.R. Alleyn, J. Bradley, R. Walker, F. Perez, **M.R. Gesinski**

ORGN **269.** Dehydrogenative cyclization of o-aminobenzyl alcohols with ketones to quinolines in water catalyzed by a water-soluble [Ir] complex. **R. Wang**

ORGN **270.** Synthesis and neoglycosylation with stereo-diverse 2-amino free-reducing sugars. **A. Scharnow**, **J. Lam**, **V. Huang**, **I. Rocroi**, C.M. Rojas

ORGN **271.** Synthesis of olefin monomers from renewable, biomass-derived polyols by catalytic deoxydehydration. **S.D. Jacob**, D. Toste

ORGN **272.** Synthesis of polyfluorinated biphenyls and polyphenyls with Buchwald phosphine ligand assisted Suzuki-Coupling. **D. Bulfield**, S. Huber

ORGN **273.** Expanding the scope of hydrogen borrowing catalysis using cyclopropyl ketones as key structural motifs. **W. Akhtar**, C. Cheong, J. Frost, N. Stevenson, T.J. Donohoe

ORGN **274.** Withdrawn.

ORGN **275.** Chemo- and enantioselective silver-catalyzed aziridinations. **M. Ju**, J.M. Schomaker

MONDAY MORNING

Section A

Moscone Center
3018/3022

Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator: Symposium in honor of Neil K. Garg

H. M. Davies, *Organizer, Presiding*

R. Sarpong, *Presiding*

8:00 ORGN **276.** Fragment coupling with carbon radicals. **L.E. Overman**

8:35 ORGN **277.** Flow chemistry on multikilogram scale. **D.D. Caspi**

9:10 ORGN **278.** Adventures with Neil Garg in distortion/interaction land. **K.N. Houk**

9:45 ORGN **279.** Engaging reactive carbocations in chemoslective and stereoselective transformations. **H. Nelson**

10:20 ORGN **280.** Complex natural products as a driving force for discovery in organic chemistry. **B.M. Stoltz**

10:55 Introduction of Awardee.

11:00 ORGN **281. Award Address** (Elias J. Corey Award for Outstanding Original Contribution in Organic Synthesis by a Young Investigator sponsored by Pfizer Endowment Fund). Recent forays in methods development and complex molecule synthesis. **N.K. Garg**

Section B

Moscone Center
3014/3016

Computer-Guided Organic Synthesis

Financially supported by Molecular Forecaster

N. Moitessier, J. Pottel, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 ORGN **282.** Computation of organic reaction pathways involving dispersion and unpaired electrons. **M. Kozlowski**

8:35 ORGN **283.** Virtual screening in asymmetric catalysis. **P. Norrby**

9:05 ORGN **284.** Simulating routine synthetic chemistry from a to z. J. Pottel, **N. Moitessier**

9:35 Intermission.

9:55 ORGN **285.** Computer guided organic synthesis. D. Walden, R.G. Carter, A.D. Smith, K. Scheidt, **P. Cheong**

10:25 ORGN **286.** From experiment to calculation and back: A round trip ride on the DFT and DFT/MM train. **F. Maseras**

10:55 ORGN **287.** Density functional theory guided catalyst design for solar generated fuels. **T. McCormick**, C. Virca

11:25 ORGN **288.** Modeling asymmetric organocatalysis. **K.N. Houk**

11:55 Concluding Remarks.

Section C

Moscone Center
3011

Biologically-Related Molecules & Processes

R. D. Broene, *Organizer*

D. Bandyopadhyay, *Presiding*

8:20 ORGN **289.** Di-substituted maleamic acid as an ultra acid-sensitive, cleavable linker for reversing the cytotoxicity pH-profile of doxorubicin in small molecule prodrugs. **M. An**, A. Zhang, L. Yao

8:40 ORGN **290.** Water-soluble NIR-absorbing rylene chromophores for biomedical applications. **K. Peneva**

9:00 ORGN **291.** Peridinin is a potent probe for the role of bilayer lipid peroxidation in pathogenesis. **A. Hill**, H. Haley, M.D. Burke

9:20 ORGN **292.** Withdrawn.

9:40 ORGN **293.** Imaging with novel catecholamine-selective fluorescent sensors. L. Zhang, X. Liu, K. Gillis, **T.E. Glass**

10:00 ORGN **294.** Synthesis and characterization of dyes for use in biological zinc-ion and reactive oxygen species dual imaging. **K. Daykin**, L. Zhu

10:20 ORGN **295.** Rational design and facile synthesis of highly modular turn-on fluorescent probe. **J.V. Jun**, D.M. Chenoweth, E.J. Petersson

10:40 ORGN **296.** Time-resolved mechanism of SpnF-catalyzed Diels-Alder reaction. **Z. Yang**, P. Yu, S. Yang, Y. Li, C. Doubleday, K.N. Houk

11:00 ORGN **297.** Synthesis of gyramide-bound photoaffinity reagents for DNA gyrase. **A.J. Kwong**, J.T. Shaw

11:20 ORGN **298.** Chemical synthesis of the potent anticancer agent prunustatin A. **M. Chojnacka**, R.A. Batey

11:40 ORGN **299.** 5-Azido-modified pyrimidine nucleosides: Chemistry and biology. **Z. Wen**, J. Peng, P. Tuttle, Y. Liang, S. Rishi, A. Adhikary, M.D. Sevilla, C. Garcia, Y. Ren, Y. Liu, S.F. Wnuk

Section D

Moscone Center
3009

Asymmetric Reactions & Syntheses

R. D. Broene, *Organizer*

Y. Chen, *Presiding*

8:00 ORGN **300.** Stereocontrolled synthesis of polypropionates based on building block assembly strategies by lithiation-borylation methodologies. **A. Millan**, B. Zhou, V.K. Aggarwal

8:20 ORGN **301.** Oxidative aerobic NHC catalysis via multistep electron transfer. **h. Sundén**, L. Ta, A. Axelsson

8:40 ORGN **302.** Chemo-enzymatic syntheses of chiral epoxides, rare sugars and flavors from levoglucosenone-derived (S)-γ-Hydroxymethyl-α,β-Butenolide (HBO). M. Moreaux, G. Bonneau, A. Peru, A. Flourat, A. Teixeira, W. Raverty, B. Greatrex, A. Haudrechy, **F. Allais**

9:00 ORGN **303.** Catalytic asymmetric alkynylation of chromenones. **L. DeRatt**, M. Pappoppula, A. Aponick

9:20 ORGN **304.** Enantioselective conjugate alkynylation enabled by Me–StackPhos. **S. Mishra**, J. Liu, A. Aponick

9:40 ORGN **305.** Developing a highly efficient, environmentally responsible alternate manufacturing process for montelukast sodium (Singulair®). **Y. Chen**, G.R. Humphrey, S.W. Krska, J. Qi, L. Tan, T. Itoh, J. Albaneze-Walker, S. Funane, T. Yokozawa, T. Kobayashi

10:00 ORGN **306.** Stereo- and enantioselective synthesis of chiral compounds bearing an all-carbon quaternary stereocenter by ZACA reaction. **S. Xu**, C. Wang, M. Komiyama, Y. Tomonari, Q. Qi, E. Negishi

10:20 ORGN **307.** Development of hydrogen-bond donor catalysts for asymmetric C-C bond formation. **M. Rombola**, V.H. Rawal

10:40 ORGN **308.** Withdrawn.

11:00 ORGN **309.** Synthesis of enantio-enriched α-quaternary prolines using a C→N→C chirality transfer. **H. Cho**, J. Shin, H. Jeon, S. Lee, S. Kim

Section E

Moscone Center
3007

Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*

T. J. Williams, *Presiding*

8:00 ORGN **310.** Tuning the regioselectivity of alkene/alkyne functionalization via a directing group strategy. **M.L. O'Duill**

8:20 ORGN **311.** Investigation of the synergistic cooperation between bimetallic systems. **S. Martínez de Salinas Uzquiza**, Á. Mudarra, M. Pérez-Temprano

8:40 ORGN **312.** N-trifluoromethylation of nitrosoarenes. **A. van der Werf**, M. Hribersek, N. Selander

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

9:00 ORGN **313.** Investigation of the organometallic chemistry of cobalt complexes: An attractive alternative to noble metals catalysts. **M. Perez-Temprano**

9:20 ORGN **314.** Palladium-catalyzed, site-selective direct allylation of aryl C–H bonds by silver-mediated C–H activation: A synthetic and mechanistic investigation. **S.Y. Lee**, J.F. Hartwig

9:40 ORGN **315.** Metal-mediated radical coupling of propargyl triflates: Acquiring a prognostic power in inter- and intramolecular reactions. **G. Melikyan**, R. Davis, E. Artashyan

10:00 ORGN **316.** Catalytic borylative opening of propargyl cyclopropane, epoxide, aziridine, and oxetane substrates: Ligand controlled synthesis of allenyl boronates and alkenyl diboronates. **J. Zhao**, K. Szabo

10:20 ORGN **317.** Visible-light radical cyclizations by photoredox/cobalt dual catalysis. **A. Casitas Montero**, M. Claros, J. Lloret-Fillol

10:40 ORGN **318.** Substrate controlled product divergence in CO_2 conversion to heterocyclic products. **J. Rintjema**, R. Epping, G. Fiorani, E. Martín, E. Escudero-Adán, A.W. Kleij

11:00 ORGN **319.** Base and solvent-free ruthenium-catalyzed alkylation of amines. J. Celaje, X. Zhang, F. Zhang, L. Kam, J.R. Herron, **T.J. Williams**

11:20 ORGN **320.** HandaPhos. A ligand enabling ppm levels of palladium in Suzuki-Miyaura couplings – the density functional theory calculations. **M. Andersson**, S. Handa, F. Gallou, J. Reilly, B.H. Lipshutz

11:40 ORGN **321.** Lewis acid-catalyzed stereoselective synthesis of cyclopenta[c]furans by a multi-component reaction. **S. Pathi Pati**, A. van der Werf, L. Eriksson, N. Selander

Section F

Moscone Center

3005

New Reactions & Methodology

R. D. Broene, *Organizer*

N. Jui, *Presiding*

8:00 ORGN **322.** Withdrawn.

8:20 ORGN **323.** Lignin depolymerization strategy using visible-light photoredox catalysis. **G. Magallanes**, C. Stephenson

8:40 ORGN **324.** Catalytic methods for heteroarene functionalization via solubility-controlled radical reactions. **N. Jui**

9:00 ORGN **325.** Photochemical aromatization: A novel approach to substituted furans and pyrroles under neutral conditions. **S. Werrel**, J. Walker, T.J. Donohoe

9:20 ORGN **326.** Site-selective aryl C-H amination via photoredox catalysis. **K. Margrey**, N. Romero, D.A. Nicewicz

9:40 ORGN **327.** Decarboxylative alkylation of biologically relevant heterocycles using photoredox catalysis. **A. Sun**, E.J. McClain, J.W. Beatty, C. Stephenson

10:00 ORGN **328.** Nanomole scale photoredox catalysis: High throughput evaluation and evolution of Ni/photoredox direct C-N amination using chemistry informer libraries. **S. Lin**, S. Dreher

10:20 ORGN **329.** Design and application of strongly reducing organic photoredox catalysts. **R.M. Pearson**, G. Miyake

10:40 ORGN **330.** Stereodivergent aminocatalytic synthesis of *Z*- and *E*- trisubstituted double bonds from alkynals. **J. Luis Barrera**, R. Mas-Balleste, J.J. Alemán

11:00 ORGN **331.** β C-H amination of alcohols via a radical relay chaperone. **E. Wappes**, K. Nakafuku, D.A. Nagib

11:20 ORGN **332.** New methodology for the synthesis of an array of bifunctional 3-hydroxy-2-pyridinone ligands for applications to therapeutic and diagnostic metal ion chelation. **C.D. Cook**, H.K. Jacobs, A.S. Gopalan

11:40 ORGN **333.** Geminal dialkyl assistance enables 5-endo-trig-type intramolecular alkene hydroarylation reactions. **X. Cai**, A. Keshavarz, J. Omaque, B.J. Stokes

Science for a Sustainable Energy Future

Energy Storage

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LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

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MONDAY AFTERNOON

Section A

Moscone Center

3018/3022

Ernest Guenther Award in the Chemistry of Natural Products: Symposium in honor of Stephen F. Martin

C. A. Maryanoff, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 ORGN **334.** Design, synthesis and biological evaluation of small-molecule inhibitors of HIV-1 entry: A potential long-term strategy for curbing the AIDS pandemic. **A.B. Smith, III**

1:55 ORGN **335.** Necessity is the mother of invention: Natural products and the chemistry they inspire. **S.E. Reisman**

2:45 ORGN **336.** Strategies and methods for chemical synthesis inspired by complex natural products. **R. Sarpong**

3:35 Introduction of Awardee.

3:45 ORGN **337. Award Address** (Ernest Guenther Award in the Chemistry of Natural Products sponsored by Givaudan Flavors Corporation). Journey from natural products to unmet medical needs in neuroscience. **S.F. Martin**

4:35 Concluding Remarks.

Section B

Moscone Center

3014/3016

Application of Physical Organic Chemistry to Challenges in Industry

G. Beutner, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 ORGN **338.** Computational study on the stereoselective reduction of a ketone intermediate with $Li(t\text{-}BuO)_3AlH$. **G.J. Tanoury**, S. Roeper

1:55 ORGN **339.** Methods and mechanism. **A.G. Doyle**

2:35 ORGN **340.** Mechanistic studies toward the development of predictive models. **A. Ramirez**

2:55 Intermission.

3:05 ORGN **341.** Development and investigation of a Pd-catalyzed C-N bond formation: Application to the synthesis of an active pharmaceutical ingredient. **J. Milne**, A. Allgeier, A. Guram, J.C. Baum, J.A. Murry, J. Colyer, X. Wang, J. Payack, T. Storz, M. Dilmeghani Seran, T. Hwang, B. Shaw

3:25 ORGN **342.** Structure-reactivity relationships in the chemistry of lithium enolates. K.A. Mack, J. Jermaks, M. Houghton, Y. Zhou, **D.B. Collum**

4:05 ORGN **343.** Application of mechanistic modeling to facilitate API process development. **D.D. Caspi**

4:25 Concluding Remarks.

Section C

Moscone Center

3011

Biologically-Related Molecules & Processes

R. D. Broene, *Organizer*

M. D. Distefano, *Presiding*

1:00 ORGN **344.** Synthesis and applications of photoactive analogues of isoprenoid diphosphates incorporating diazirines. J.S. Vervacke, A. Sarkis, A.L. Funk, E.L. Lorimer, C. Hrycyna, C.L. Williams, **M.D. Distefano**

1:20 ORGN **345.** Development of synthetic methods for the preparation of biologically active compounds. **A.R. Angeles**

1:40 ORGN **346.** Synthesis and biological evaluation of novel heterocyclic scaffolds as infectious disease lead compounds. **G.A. Edwards**, J.G. Pierce

2:00 ORGN **347.** Strain induced couplings mediated by visible light. **J.D. Weaver**, K. Singh

2:20 ORGN **348.** Withdrawn.

2:40 ORGN **349.** Zwitterionic pyrrolidine-phosphonates: Transition state mimics of the glycoside hydrolase-like phosphorylase *Streptomyces coelicolor* GlgEI-V279S. S. Veleti, C. Petit, D.R. Ronning, **S.J. Sucheck**

3:00 ORGN **350.** Chemosynthetic livers: Predict, prepare and prove the structure, activity and toxicity of drug metabolites. R. Chorghade, **M. Chorghade**

3:20 ORGN **351.** Chemosynthetic livers: Evaluating plausible drug-drug interactions relating to metabolite suppression or attenuation. **R. Chorghade**, M. Chorghade

3:40 ORGN **352.** Designing foldamers: Synthesis of hydrophilic peptoids that fold in a predictable manner. **P.W. Peterson**, J.G. Schmidt, A.S. Anderson, R.D. Gilbertson, R.F. Williams, C.E. Strauss

4:00 ORGN **353.** Origin of RNA: Model studies for the prebiotic synthesis of nucleosides. **G. Purushothaman**, R. Breslow

Section D

Moscone Center

3009

Asymmetric Reactions & Syntheses

R. D. Broene, *Organizer*

G. R. Boyce, *Presiding*

1:00 ORGN **354.** Ruthenium catalyzed C-C coupling of alcohols with alkynes and 1,3-enynes *via* hydrogen transfer. **K.D. Nguyen**, D. Herkommer, T. Liang, B.Y. Park, M.J. Krische

1:20 ORGN **355.** Withdrawn.

1:40 ORGN **356.** Why is asymmetric hydrogenation of 3-substituted pyridinium salts so problematic? **J.G. De Vries**, M. Renom-Carrasco, P. Gajewski, L. Lefort, L. Pignataro, U. Piarulli, C. Gennari

2:00 ORGN **357.** Asymmetric synthesis of drug candidates: Discovery and development of novel aza-Michael catalysts for the synthesis of Letermovir. **S. Dalby**

2:20 ORGN **358.** Brønsted acid–hydrogen bonding model for cinchona alkaloid-catalyzed asymmetric conjugate addition reactions. **M.N. Grayson**, K.N. Houk

2:40 ORGN **359.** Electrostatic interactions control the selectivity of NHC-catalysed kinetic resolution. **R. Maji**, S.E. Wheeler

3:00 ORGN **360.** Site selective and stereoselective functionalization at primary, secondary and tertiary C-H bonds. H.M. Davies, **K. Liao**

3:20 ORGN **361.** Efforts towards the concise stereoselective synthesis of thujone. **G.R. Boyce**

Section E

Moscone Center

3007

Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*

L. M. Stanley, *Presiding*

1:00 ORGN **362.** Designing Pd-NHC complexes to provide selective monoarylation. **M.G. Organ**

1:20 ORGN **363.** Designing catalysts for the selective coupling of secondary alkylzinc reagents. **M.G. Organ**

1:40 ORGN **364.** Ether solvated lithium pinacolone enolates: Solution and solid state characterizations. **O. Tai**, P.G. Williard

2:00 ORGN **365.** Template assisted remote C–H bond functionalizations. **A. Maji**, D. Maiti

2:20 ORGN **366.** Think outside the box – air-stable paraffin pellets with highly active and selective Mo- & W-catalysts for industrial and everyday use in olefin metathesis. **L. Ondi**, J.B. Czirok, A. Bucsai, J. Varga, C. Hegedus, C. Gego, V. Botka, J. Csernak, G.E. Frater

2:40 ORGN **367.** Studies toward copper-mediated [^{18}F]radiofluorination of arylstannanes. **K.J. Makaravage**, A.F. Brooks, A. Mossine, M.S. Sanford, P.J. Scott

3:00 ORGN **368.** Conformational flexibility as a design element in ligand design for palladium-catalyzed bond-forming reactions. **K.H. Shaughnessy**

3:20 ORGN **369.** Rhodium-catalyzed asymmetric 1,4-addition of α,β-unsaturated imino esters using chiral bicyclic bridgehead phosphoramidite ligands. **H. Kim**, A. Lee

3:40 ORGN **370.** Nickel-catalyzed carboacylation of alkenes via activation of amide C-N bonds. J.A. Walker, K.L. Vickerman, J. Humke, **L.M. Stanley**

4:00 ORGN **371.** Foldamer synthesis using the Ruthenium-Catalyzed Azide Alkyne Cycloaddition (RuAAC) reaction. J.R. Johansson, A. Said Stålsmeden, T. Beke-Somfai, **N. Kann**

4:20 ORGN **372.** Development of an efficient synthesis of an inhaled drug candidate. **D. Steinhuebel**

Section F

Moscone Center

3005

New Reactions & Methodology

R. D. Broene, *Organizer*

M. D. Clift, *Presiding*

1:00 ORGN **373.** Catalytic asymmetric synthesis of pyrrolidines and piperidines. L. Pilsl, T. Ertl, J. Yedoyan, **O. Reiser**

1:20 ORGN **374.** Withdrawn.

1:40 ORGN **375.** New reactions inspired by cofactor-mediated transformations. **M.D. Clift**

2:00 ORGN **376.** N-cyanation of secondary amines using trichloroacetonitrile. **L.C. Morrill**, J. Ayres, K. Ling

2:20 ORGN **377.** Additive-free chemoselective reductions of phosphine oxides. **J. Buonomo**, C. Eiden, C.C. Aldrich

2:40 ORGN **378.** Recent advances in phosphine oxide catalysis. **P.H. Toy**

3:00 ORGN **379.** Cheap, recyclable trifluoromethylation reagents from fluoroform. **J.B. Geri**, N.K. Szymczak

3:20 ORGN **380.** Novel synthesis of fluorinated indoles and benzofurans via oxidative dearomatization. **D. Smith**, E. Vitaku, J.T. Njardarson

3:40 ORGN **381.** Radical chlorodifluoromethylation: Providing a versatile motif for (hetero)arene diversification. **R.C. McAtee**, C. Stephenson

4:00 ORGN **382.** Efficient Formal Intramolecular Diels-Alder (FIMDA) cyclization of electron-deficient dienynes. **N. Kramer**, G.B. Dudley

4:20 ORGN **383.** Alkyne chemistry for the synthesis of high-value molecular targets. **G.B. Dudley**

4:40 ORGN **384.** Synthesis of N-sulfonyl amidines through $Mo(CO)_6$ catalyzed amide reduction to enamines. **P. Trillo**, H. Adolfsson

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

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ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

S. M. Silverman, *Organizer*

8:00 - 10:00

106, 118, 126-127, 129, 140-141, 143-144, 147, 151-152, 159, 163-164, 166-167, 173, 178, 193-194, 196, 204, 212, 214, 222, 224, 228, 232, 234, 242, 247-248, 252, 254, 261, 270-271. See previous listings.

502, 514, 529-530, 532, 537, 548, 554, 556-557, 581, 586, 594, 602, 606, 608, 611, 614, 618, 736, 740, 753, 763, 772, 797, 810, 816, 822, 825-829, 833-834, 836, 839, 841, 843-844. See subsequent listings.

TUESDAY MORNING

Section A

Moscone Center

3018/3022

ACS Award for Creative Work in Synthetic Organic Chemistry: Symposium in honor of Matthew S. Sigman

J. Aube, *Organizer, Presiding*

8:00 ORGN **385.** Searching for selective catalytic reactions in complex molecular environments. **S.J. Miller**

8:45 ORGN **386.** Development and applications of new fluorination methods. **M.S. Sanford**

9:30 ORGN **387.** Organic reactions inspired by the organometallic chemistry of gold. **D. Toste**

10:15 Intermission.

10:25 ORGN **388.** New directions in Ni-catalyzed cross coupling. **A.G. Doyle**

11:10 Introduction of Awardee.

11:15 ORGN **389. Award Address** (ACS Award for Creative Work in Synthetic Organic Chemistry sponsored by MilliporeSigma). Enantioselective formation of remote chiral centers through Pd-catalyzed alkene functionalization. **M.S. Sigman**

Section B

Moscone Center

3014/3016

Advances in Organic Synthesis: Successes from Academia-Industry Partnerships

L. C. Campeau, *Organizer*

T. Lyons, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN **390.** Academic-industry collaborations at Merck process research & development: Working with partners to enable scientific excellence. **R. Ruck**

8:45 Discussion.

8:50 ORGN **391.** Pharmaceutical applications of visible light photoredox catalysis. **C. Stephenson**

9:30 Discussion.

9:35 ORGN **392.** Collaborative academic/industrial research under the umbrella of the NSF Center for selective C-H functionalization. **H.M. Davies**

10:15 Discussion.

10:20 Intermission.

10:30 ORGN **393.** From bench to bottle and the relationships in between. **S.L. Trice**

11:10 Discussion.

11:15 ORGN **394.** Practical aerobic (and electrochemical) oxidation reactions. **S.S. Stahl**

11:55 Concluding Remarks.

Section C

Moscone Center

3011

Heterocycles & Aromatics

R. D. Broene, *Organizer*

G. R. Geier, *Presiding*

8:00 ORGN **395.** Practical design and synthesis of Merestinib's *N*1-methylindazole building block. **Y. Lu**, K.P. Cole, J. Fennell, J. Burt, T.D. Maloney, D. Mitchell

8:20 ORGN **396.** Synthesis of medium-sized rings and cyclic tripeptides through ring expansion of amino-imides. R. Mendoza-Sanchez, **V. Corless**, N.N. Nguyen, D.J. Tantillo, A.K. Yudin

8:40 ORGN **397.** Toolbox of porphyrins, phthalocyanines, and other porphyrinoids. **C.M. Drain**, N. Bhupathiraju, W. Rizvi

9:00 ORGN **398.** Synthesis of bacteriochlorins with an isocyclic ring: The skeleton of bacteriochlorophylls. **S. Zhang**, J.S. Lindsey

9:20 ORGN **399.** More studies on cyclic six- and seven-membered 2,3-diaryl-1,3-thiaza-4-ones. **L.J. Silverberg**, H. Yennawar, C.N. Pacheco, A.F. Lagalante, H.F. Sobhi, K. Alemany, J. Bachert, L. Baker, K. Bandholz, J.A. Bayliff, R. Bendinsky, H.G. Bradley, M.J. Buchwalter, A. Cali, O.A. Cardenas, L. Chen, B.K. Colburn, A.D. Cooper, D.J. Coyle, J.R. Dahl, M. Felty, R.F. Fox, J.M. Islam, E. Kimmel, S.E. Koperna, M.K. Lawler, Q.J. Moyer, C.R. Mroz, D.J. Noble, K.C. Perhonitch, H.E. Reppert, H. Singh, C.R. Verhagen, R.M. Vidal, A. Weisbeck, Y. Xie, Z. Yang

9:40 ORGN **400.** Two-step, one-flask synthesis of an N-confused porphyrin bearing pentafluorophenyl substituents. J.M. Fisher, V.K. Kensy, **G.R. Geier**

10:00 ORGN **401.** Porphyrins as functional scaffolds for 2D and 3D materials. **M.O. Senge**

10:20 ORGN **402.** Genuine diversity in short order: Development and application of facile [2+2+2] cyclotrimerisation methodology suitable for medicinal chemistry. S. Peace, **C.J. Tame**, C. Jamieson, G. Inglis, G. Vitulli, N. Wellaway, N. Anderson, A. Bouisseau, T.D. Sheppard, H. Hailes, R. Foster

10:40 ORGN **403.** Synthesis, functionalization, and reactivity of novel silicon-containing heterocycles for drug discovery. **S. Barraza**, S.E. Denmark

11:00 ORGN **404.** Synthesis of functionalized polyphenylene dendrimers. **A. Baun**, A. Narita, K. Muellen

11:20 ORGN **405.** Evaluating regioselectivity outcomes in 5-endo-trig and 6-endo-trig hydroarylation reactions of β-benzylstyrenes and β-homobenzylstyrenes. **A. Keshavarz**, X. Cai, L.N. Kagiri, B.J. Stokes

Section D

Moscone Center

3009

Molecular Recognition & Self-Assembly

R. D. Broene, *Organizer*

E. Fatila, *Presiding*

8:00 ORGN **406.** Functional integration of abiotic triazine-derivatives with DNA and RNA. **D. Bong**

8:20 ORGN **407.** Phenylacetylene oligomers as synthetic information molecules. **J. Swain**, C. Hunter

8:40 ORGN **408.** Selective recognition and separation of oxoanions using a guanidinium ligand. **C. Seipp**, N.J. Williams, V. Bryantsev, A. Ivanov, B.A. Moyer, R. Custelcean

9:00 ORGN **409.** Multidentate halogen bonding organocatalysts in molecular recognition studies. **S. Huber**, S.H. Jungbauer, D. Bulfield, S. Schindler, F. Kniep, E. Herdtweck, C. Lehmann, S. Keller, A. Linke, S.R. Waldvogel

9:20 ORGN **410.** Binding anions using a clamshell based receptor. **E. Fatila**, E.B. Twum, J.A. Karty, K.P. McDonald, A.H. Flood

9:40 ORGN **411.** Self-assembly of Star of David: 2D and 3D approaches. **B. Song**, **Z. Zhang**, **X. Li**

10:00 ORGN **412.** Location of the steric speed bump controls squaraine threading by tretralcation macrocycle. **C.F. Gomez**, W. Liu, M. Betancourt, B.D. Smith

‡*Cooperative Cosponsorship*

10:20 ORGN **413.** Pumping potassium against concentration gradient through unimolecular channel. **J. Hou**

10:40 ORGN **414.** Sensing of chiral compounds via self-assembly with a stereodynamic probe. **Z. De los Santos**, C. Wolf

11:00 ORGN **415.** Dynamic peptides as biomimetic carbohydrate receptors. **B. Ravoo**

11:20 ORGN **416.** Highly selective biomimetic artificial K^+ channels. **M.D. Barboiu**

11:40 ORGN **417.** Driving assembly of cyanostar with hydroxyanions. **E. Fatila**, E.B. Twum, A. Sengupta, M. Pink, J.A. Karty, K. Raghavachari, A.H. Flood

Section E

Moscone Center

3007

Metal-Mediated Reactions & Syntheses

R. D. Broene, *Organizer*

C. W. Alexander, *Presiding*

8:00 ORGN **418.** Phosphine-ligated alkylpalladium(II) amido complexes: Understanding the kinetic barrier to reductive elimination of alkylamines. **D.M. Peacock**, J.F. Hartwig, Q. Jiang, T.R. Cundari

8:20 ORGN **419.** Consecutive multicomponent syntheses of pyrazoles-diversity-oriented approach to blue emitters and emission solvatochromic dyes. **T.J. Muller**, A.C. Goetzinger, M. Denissen

8:40 ORGN **420.** Chemo- and stereoselective rhodium-catalyzed ene-cycloisomerization of thioether-substituted alkenylidenecyclopropanes: Metal-mediated β-sulfide migration. **Y. Su**, P. Evans

9:00 ORGN **421.** Earth abundant catalysts for the hydrofunctionalization of unsaturated compounds. **C.C. Eichman**, S. Lee, A.J. Villani-Gale

9:20 ORGN **422.** Pd-catalyzed fluorination of (hetero)aryl halides and triflates. **P.J. Milner**, S.L. Buchwald

9:40 ORGN **423.** New catalytic methods for N-heterocycle synthesis by late transition metal-mediated C-H bond activation. **P. Kilaru**, P. Zhao

10:00 ORGN **424.** Investigating reactivity, structure and reusability of an insoluble iridium catalyst for C-H borylations. **C.R. Jayasundara**, R.E. Maleczka, M.R. Smith, J. Oppenheimer

10:20 ORGN **425.** Catalytic asymmetric hydroboration of internal alkenes. **Y. Xi**, J.F. Hartwig

10:40 ORGN **426.** New transition metal-catalyzed reductive processes using H atoms from water mediated by tetrahydroxydiboron and related reagents. S. Cummings, T. Le, L. Quiambao, A. Brito, J. Alvarenga, **B.J. Stokes**

11:00 ORGN **427.** Chemoselective CuAAC reactions via shifting the rate-determining step: Orthogonal reactivity of aromatic ynamines. **C.P. Seath**, G.A. Burley, A.J. Watson

11:20 ORGN **428.** Hydrogen borrowing catalysis: Strategic application and transformation of *ortho*-disubstituted and cyclopropyl ketones. **J. Frost**, C. Cheong, W. Akhtar, T.J. Donohoe

11:40 ORGN **429.** Methods for the synthesis of α,β-substituted vinyl phosphonates from novel α-phosphonovinyl triflates. **C.W. Alexander**

Section F

Moscone Center

3005

New Reactions & Methodology

R. D. Broene, *Organizer*

W. Santos, *Presiding*

8:00 ORGN **430.** Developing the phosphinoboration reaction. **S.A. Westcott**, S.J. Geier, C.M. Vogels, N.R. Mellonie, S. Doherty

8:20 ORGN **431.** Understanding and exploiting selectivity in the Ir-catalysed C-H borylation of heterocycles. A. Hones, J. Wright, D. Blakemore, **P.G. Steel**

8:40 ORGN **432.** Diastereoselective $B(C_6F_5)_3$-catalyzed reductive carbocyclization of unsaturated carbohydrates. **J.A. Dabrowski**, T.A. Bender, H. Zhong, M.R. Gagne

9:00 ORGN **433.** Diastereoselective borocyclopropanation of allylic ethers using a boromethylzinc carbenoid. **G. Benoit**, A.B. Charette

9:20 ORGN **434.** Insights in dehydrogenative borylation reactions. E. Romero, **R. Jazzar**, G. Bertrand

9:40 ORGN **435.** Rapid access to an antimalarial drug core via a three-component minisci reaction. **J. Lear**, D.A. Nagib

10:00 ORGN **436.** Open-to-air hydroboration of alkenes and alkynes with ammonia borane. **A.S. Kulkarni**, M.P. Drolet, H.A. Jawale, P.V. Ramachandran

10:20 ORGN **437.** One-pot regioselective synthesis of highly functionalized chromone derivatives. **R. Bam**, W. Chalifoux

10:40 ORGN **438.** Transition metal-free activation and intramolecular *trans* diboration of propargylamides using unsymmetrical diboron. **W.L. Santos**, R. Snead, F. Astha, Y. Dai

11:00 ORGN **439.** Regioselective boracarboxylation of vinyl arenes. **B.V. Popp**

11:20 ORGN **440.** Visible light-mediated synthesis of 1-aminonorbornanes, a new saturated building block for drug discovery. **D. Staveness**, T. Sodano, C. Stephenson

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡

TUESDAY AFTERNOON

Section A

Moscone Center

3018/3022

James Flack Norris Award in Physical Organic Chemistry: Symposium in honor of Robert A. Moss

J. Lee, *Organizer*

M. Platz, *Presiding*

1:00 Introductory Remarks.

1:05 ORGN **441.** Origin of homochirality in amino acids and sugars, and enzyme-like catalysis, under prebiotic conditions. **R. Breslow**

1:30 ORGN **442.** All happens at the interface: Monolayer-protected gold nanoparticles and beyond. **P. Scrimin**

1:55 ORGN **443.** Gas phase studies of catalysis. **J.K. Lee**

2:20 Intermission.

2:30 ORGN **444.** Sigma-electron delocalization: Why are loose oligosilane helices strongly conjugated and tight helices not at all? M. Jovanovic, D. Antic, **J. Michl**

2:55 ORGN **445.** What is the effect of the replacement of CH_2 by O on the measured and calculated values of the singlet-triplet energy difference (ΔE_{ST}) in trimethylenemethane (TMM), oxyallyl (OXA), dehydroacetic acid (DHAA), and carbon trioxide (CO_3)? **W.T. Borden**, X. Wang, B. Chen, D.A. Hrovat

3:20 ORGN **446.** Valley of fear(lessness): Carbene mysteries. **D.C. Merrer**

3:45 Intermission.

3:55 Introduction of Awardee.

4:00 ORGN **447. Award Address** (James Flack Norris Award in Physical Organic Chemistry sponsored by the ACS Northeastern Section). Complexes and activation parameters in carbene-alkene additions. **R.A. Moss**

4:50 Concluding Remarks.

Section B

Moscone Center

3014/3016

Advances in Organic Synthesis: Successes from Academia-Industry Partnerships

L. C. Campeau, T. Lyons, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 ORGN **448.** Iron and cobalt catalysis at the academic-pharma interface. **P.J. Chirik**

1:45 Discussion.

1:50 ORGN **449.** Stereoselective formation of tetrasubstituted olefins via enol tosylate formation. A. McClory, D.B. Collum, T. Cravillion, F. Gosselin, C. Han, D. Le, B. Li, N. Lim, K.A. Mack, S. Savage, **H. Zhang**

2:30 Discussion.

2:35 ORGN **450.** Kinetic and mechanistic studies in support of process research and development. **D.G. Blackmond**

3:15 Discussion.

3:20 Intermission.

3:30 ORGN **451.** Strain-release amination. **M.R. Collins**, R. Gianatassio, J.M. Lopchuk, J. Wang, C. Pan, L. Malins, L. Prieto, T.A. Brandt, G. Gallego, N. Sach, J. Spangler, P. Zhu, J. Zhu, P.S. Baran

4:10 Discussion.

4:15 ORGN **452.** Dow/UM collaboration on halex fluorination. **M.S. Sanford**

4:55 Concluding Remarks.

Section C

Moscone Center

3011

Heterocycles & Aromatics

R. D. Broene, *Organizer*

J. Day, *Presiding*

1:00 ORGN **453.** Functionalized tunable aryl alkyl ionic liquids. **M. Kaliner**, T. Strassner

1:20 ORGN **454.** Thiophene-based double helix shaped molecules. **H. Wang**

1:40 ORGN **455.** Oligodithienothiazines – electronrich heterocyclic oligomers with red-shifted solution and solid-state luminescence. **T.J. Muller**, J. Nau, C. Dostert

2:00 ORGN **456.** DNA binding studies of Schiff base heterocyclic derivatives: *In vitro* antibacterial and antioxidant assessment. **R. Uddin**, R. Arif

2:20 ORGN **457.** Panel of dimethylamino flavylium cyanine dyes spanning the NIR-I and NIR-II regions. **E.D. Cosco**, J.R. Caram, O. Bruns, T.M. Swager, M.G. Bawendi, E.M. Sletten

2:40 ORGN **458.** Challenges and opportunities for synthetic methodology in fragment-based drug discovery. **J. Day**

3:00 ORGN **459.** Novel approaches to nitrogen-containing heterocycles. **P.D. Parker**, J.G. Pierce

3:20 ORGN **460.** Synthesis and biological evaluation of A_3B phthalocyanines for photodynamic therapy and imaging. **E. Okoth**, M. Mathis, G. Vicente

3:40 ORGN **461.** Solvent controlled regioselective reversal in N-alkylation reactions of fused-ring azole heterocycles including pyrazolo[3,4-*d*] pyrimidines, purines, [1,2,3]triazolo[4,5-*d*] pyrimidines and related deaza-compounds. **B.C. Bookser**, M.I. Weinhouse, A.C. Burns, A.N. Valiere, B. Dyck, L.J. Valdez, A.L. Rheingold, C.E. Moore

4:00 ORGN **462.** Synthesis of catenane-like paddle wheel structures. **B. Dumslaff**, A. Narita, K. Muellen

4:20 ORGN **463.** Modular synthesis and tuning of antiaromaticity of novel π-systems containing cyclobutadienoids. **Z. Jin**, Y. Xia, L. Chen

4:40 ORGN **464.** Copper-catalyzed cyclic ether synthesis *via* addition of alkyltrifluoroborates to alkenols. **C. Um**, S.R. Chemler

Section D

Moscone Center

3009

Molecular Recognition & Self-Assembly

R. D. Broene, *Organizer*

R. Khaliullin, *Presiding*

1:00 ORGN **465.** Self-assembly of metal-terpyridine complexes in the presence of cucurbit[n]uril. **M. Raeisi**, E. Masson

1:20 ORGN **466.** Self-sorted multi-component photoconductive gels. **E. Draper**, J.R. Lee, A.J. Cowan, D.J. Adams

1:40 ORGN **467.** Study of four simultaneously dynamic covalent reactions: Experimental proof of reversibility and orthogonality. **H. Seifert**, K. Ramirez Trejo, E.V. Anslyn

2:00 ORGN **468.** Developing a non-invasive monitoring system using near IR dyes. **H. Sepasizangabadi**, N.P. Cooley, X. Shao, T.E. Glass

2:20 ORGN **469.** Binding studies and organocatalytic activity of a preorganized bidentate halogen bonding molecule. **A. Riel**, J. Sun, C. Massena, O.B. Berryman

2:40 ORGN **470.** Synthesis and study of new highly soluble tetraalkylated bis(imino) guanidiniums for the selective removal of oxoanions from aqueous solutions containing mixtures of anions. **N.J. Williams**, C. Seipp, K.A. Garrabrant, R.J. Ellis, R. Custelcean, B.A. Moyer

3:00 ORGN **471.** Russian nesting doll complexes of molecular baskets and zinc containing TPA ligands. **Z. Lei**, S. Polen, C.M. Hadad, **T. Rajanbabu**, J.D. Badjic

3:20 ORGN **472.** Synthesis and metal binding of azole-containing peptidomimetics. A.A. Fuller, **A. Mohan**, C. Bosmajian

3:40 ORGN **473.** Stopper group steric effects on macrocycle encapsulation of indolenine squaraine dyes. **T. Jarvis**, W. Liu, B. Smith

4:00 ORGN **474.** Self-assembly of 3D columnar structures and 2D bilayers through antimony(III) secondary bonding interactions. S. Moaven, J. Yu, J. Yasin, **A.F. Cozzolino**

4:20 ORGN **475.** Thermally stable triazine-based organic superstructure. **S. Jung**, J. Baek

4:40 ORGN **476.** Two similar steroid hormones – drastically different complexation behavior: How structural nuances control interactions with aromatic electron density. Z. Luo, T. Friscic, **R. Khaliullin**

Section E

Moscone Center

3007

Total Synthesis of Complex Molecules

R. D. Broene, *Organizer*

L. E. Sirois, *Presiding*

1:15 ORGN **477.** Efforts towards the total synthesis of maoecrystal V. **B.R. Smith**, J.T. Njardarson

1:35 ORGN **478.** Withdrawn.

1:55 ORGN **479.** Total synthesis of lauralline. **T. Okada**, F. Yoshimura, K. Tanino

2:15 ORGN **480.** Total synthesis of (-)-virosaine A. **J. Hughes**, J. Gleason

2:35 ORGN **481.** Kilogram-scale synthesis of RORc ligand GDC-0022. **L.E. Sirois**, D. Lao, J. Xu, R. Angelaud, F. Gosselin

2:55 ORGN **482.** Toward total syntheses of cryptobeilic and isocryptobeilic acid D. **L. Kim**, E. Go, S. Wetzler, K.J. Kron, G.E. Miller, D.A. Vosburg

3:15 ORGN **483.** Synthetic progress towards the total synthesis of mandelalide B. **A. Ghosh**, J. Li, N. Veerasamy, R.G. Carter

3:35 ORGN **484.** Progress toward the total synthesis of anticancer deoxypodophyllotoxin and antiviral F4-4. **D.I. Saavedra**, B. Rencher, P.J. Hurst, M. Andrus

3:55 ORGN **485.** Progress towards the first total synthesis of undulifoline. **T.M. Williams**, C. Stephenson, E. Swift

4:15 ORGN **486.** 14-Step total synthesis of thapsigargin from (*R*)-(–)-carvone. **D. Chen**, P. Evans

Section F

Moscone Center

3005

New Reactions & Methodology

R. D. Broene, *Organizer*

W. M. Braje, *Presiding*

1:00 ORGN **487.** Frustrated Lewis pair hydrogenation of *a,b*-unsaturated carbonyl compounds. **I. Khan**, L.C. Morrill

1:20 ORGN **488.** Stereoselective synthesis of tetrasubstituted olefins via mild, one-pot syn-elimination approach. **N. Lim**, P. Weiss, X. Li, H. Zhang, F. Gosselin

1:40 ORGN **489.** Tandem chemoselective Suzuki-Miyaura cross-coupling enabled by nucleophile speciation control. **C.P. Seath**, A.J. Watson

2:00 ORGN **490.** Palladium-catalyzed alkoxycarbonylation of unactivated alkyl bromides. **B.T. Sargent**, E.J. Alexanian

2:20 ORGN **491.** Recent advances in nickel-catalyzed activation of amides. **E.L. Baker**, N.K. Garg

2:40 ORGN **492.** Gold catalysis for the construction of barbaralones and related polycyclic caged frameworks. **S. Ferrer Cabrera**, A.M. Echavarren

3:00 ORGN **493.** Iron(III)-catalyzed carbonyl-olefin metathesis. **C. Schindler**

3:20 ORGN **494.** Nickel catalyzed reductive cross-electrophile couplings to furnish cyclopropanes. **T. Endean**

3:40 ORGN **495.** Investigations in the mechanism of metal-catalyzed hydroarylation. **A.J. Villani-Gale**, S. Phan, S. Lee, J.J. Devery, C.C. Eichman

4:00 ORGN **496.** Rhodium-catalyzed oxidative (4+2) annulations of *o*-alkenylanilides. **A. Seoane**, C.C. Comanescu, X. Diz, J.L. Mascarenas, M. Gulias Costa

4:20 ORGN **497.** Recent advances in the transition metal-catalyzed decarboxylative generation and alkylation of 2-azaallyl anions. **J.J. Chruma**, S. Tang, X. Wang, Q. Lin, M. Li, P.J. Walsh, S. Wang, X. Qian

4:40 ORGN **498.** Organic chemistry in water: Applications in the pharmaceutical industry. **W.M. Braje**, J. Kaschel, J. Klee, T. Lindner, K. Britze, A. Jolit, J. Dietrich

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡

TUESDAY EVENING

Section A

Moscone Center

Hall D

Advanced Materials Technologies, Systems & Processes

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **499.** Tough aqua material for a tough application: Self-assembled membrane for water purification sustaining high pressures. **E. Cohen**, H. Weissman, E. Shimoni, I. Kaplan-Ashiri, K. Werle, W. Wohlleben, B. Rybtchinski

ORGN **500.** Enhanced light extraction efficiency of OLEDs by quasi-periodic diffractive nanogratings. **Y. Jeong**

ORGN **501.** Unsymmetrical effect of Hexa-peri-hexabenzocoronenes on columnar mesophase behavior stability. **H. Chen**

ORGN **502.** Post functionalization of polycarboxy fantrip. **R. Gilley**, W.B. Thompson, B.T. King

Section B

Moscone Center

Hall D

Biologically-Related Molecules & Processes

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **503.** Fast track process research: Identification and development of highly improved routes to GDC-0810. **T. Cravillion**, A. McClory, S. Savage, N. Lim, H. Zhang, C. Han, F. Gosselin

ORGN **504.** Development of an expedient synthesis to GDC-0853: A reversible Bruton's tyrosine kinase inhibitor. **N. Lim**, T. Cravillion, D. Beaudry, J. Defreese, Q. Tian, H. Zhang, F. Gosselin

ORGN **505.** Expedient and modular access to [6,5]- and [6,6]-2-azabicyclic morpholinones by iron- or palladium-catalyzed intramolecular coupling of vicinally functionalized alcohol-bearing allylic lactams. **K. Hovenkotter**, T. Beng

ORGN **506.** Synthesis, chemical reactivity, and medicinal activity of novel chiral piperidines. **H. Braunstein**, T. Beng

ORGN **507.** Cleavable fluorescent probes for direct measurement of nutrient uptake. **V. Begoyan**, M. Tanasova

ORGN **508.** Synthesis of oligodeoxynucleotides containing electrophilic groups. **S. Shahsavari**, X. Lin, J. Chen, N. Green, D. Goyal, S. Fang

ORGN **509.** Epoxyisoindoline formation through tandem Ugi-Smiles Diels-Alder reactions. **P.E. Alabi**, S. Luesse

ORGN **510.** Development of a tandem oxy-Michael Ugi-Smiles reaction. **R. Ayres**, S. Luesse

ORGN **511.** Investigation and synthesis of isoform-selective histone deacetylase inhibitors. **M.J. O'Neill**, O. Wiest, P. Helquist

ORGN **512.** Photocaged NAD^+ for mechanistic investigations of HMG-CoA reductase. **F. Salahi**, O. Wiest, P. Helquist, C. Stauffacher, V. Purohit, T. Quinn

ORGN **513.** Synthesis and biological evaluation of inhibitors of KasA indentified through virtual screening: A novel inhibitor of *Mycobacterium tuberculosis*. **D. Oldham**, A. Priest, G. Henry, L. Lewis, D. Toth

ORGN **514.** Synthesis of oxidative metabolites of the persistent organic pollutant DEHP. **K. McDaniel**, D. Oldham

ORGN **515.** Practical and concise synthesizes of antifungal amphiphilic kanamycin analogs. **M. Alfindee**, Q. Zhang, J.P. Shrestha, V.d. Nziko, Y. Kawasaki, X. Peng, J. Takemoto, C.T. Chang

ORGN **516.** Toward the total syntheses of natural products containing trans-decalin skeleton from masked o-benzoquinone. **M. Li**, H. Shiao, H. Hsieh

ORGN **517.** Synthesis of photocyclization/oxidation-based fluorophores for cell and tissue imaging. **S. Suh**, D.M. Chenoweth

ORGN **518.** DNA compatible nitro reduction and benzimidazole synthesis. **H. Du**, H. Huang

ORGN **519.** PBr_3-mediated unexpected reductive deoxygenation of α-aryl-pyridinemethanols: Synthesis of arylmethylpyridines toward EP_1 antagonists. **S. Seto**, Y. Nishigaya, K. Umei, D. Watanabe, Y. Kohno

ORGN **520.** Efficient cross metathesis of allyl sulfones with isoprenoids for the synthesis of fluorescent lipid probes. **R. Sapkota**, J. Jarvis, N. Paz, T. Schaub, J.B. Arterburn

ORGN **521.** Towards understanding of peroxidation of mammalian sterols: Microwave-assisted synthesis of 7-dehydrocholesterol isomers. **A.C. Olvera**, **J. Ramos Flores**, H. Muchalski

ORGN **522.** Synthesis of 6-substituted dopamine derivatives. **J.A. Rogowiec**, K. Reed, J. Rote, M.L. Cafiero, L.W. Peterson

ORGN **523.** Schiff bases and hemiaminals: Synthesis, mechanism of formation and biological evaluation. **M. Islam**, M.R. Karim

ORGN **524.** Synthesis and atropisomeric binding of novel β-carbolines to brain receptors. **C. Foley**, S.P. Mulcahy

ORGN **525.** Design and synthesis of halogen bonding compounds for the inhibition of IGPs. **J.M. Ellsworth**, C.C. Browder

ORGN **526.** Synthesis and characterization of a verdazyl radical labeled amino acid spin probe. D.J. Brook, **A. Clemens**, **J. DaRos**

ORGN **527.** Shake it off: Ring expanded sugars as ligands for the *E. coli* lectin FimH. R. Vannam, P. Zihlmann, B. Fiege, C. Sager, S. Rabbani, R.P. Jakob, R. Preston, A. Zalewski, T. Maier, B. Ernst, **M.W. Peczuh**

ORGN **528.** Targeting infectious diseases with dihydropyrimidinone-derived chemotypes. **M. DiCairano**, R. Trilles, S. Schaus, L. Brown

ORGN **529.** Light induced cell migration *in vivo* with photocaged TLR agonist. **K. Ryu**, B. McGonnigal, A.P. Esser-Kahn

ORGN **530.** Synthesis and evaluation of a novel class of androgen receptor signaling axis inhibitors targeting castration-resistant prostate cancer. **D. N G Ralalage**, J. An, M.B. Rettig, M.E. Jung

ORGN **531.** Synthesis of oligonucleotides containing C8-2'-deoxyguanosine adduct of the tobacco carcinogen 2-amino-9H-pyrido [2, 3-b] indole (AαC). **A. Chatterjee**, A.K. Basu

ORGN **532.** Synthesis of 4-N-alkyl gemcitabine analog bearing β-keto tosylate moiety suitable for ^{18}F-labeling. **M. Cabrera**, C. Gonzalez, N. Sulimoff, S.F. Wnuk

ORGN **533.** Development of amino acid-based inhibitors against Aspartate-N-Acetyltransferase (ANAT) for the treatment of Canavan disease. **V. Mutthamsetty**, B. Thangavelu, Q. Wang, R.E. Viola

ORGN **534.** Stepwise two-photon activatable BODIPY for multi-channel imaging in developing embryos. **D. Herrera**, Y. Zhang

ORGN **535.** Fluorescent probes for targeting fructose transport. **J. Fedie**, S. Xia, M. Tanasova

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ORGN **536.** Increasing the therapeutic index for head-and-neck squamous cell carcinoma targeted therapy through the derivatization of deoxynyboquinone. **J.E. Jurczyk**

ORGN **537.** Tandem incorporation of enantiomeric residues engenders discrete peptoid structures. **E.M. Mumford**, B.C. Gorske, R.R. Conry

ORGN **538.** Co-bisintercalating FRET-based fluorescent bottlebrush polymer nanotags. **M. Evanoff**, M. Fouz, B.A. Armitage

ORGN **539.** Computational modeling of PikC activity and selectivity for guided protein and substrate engineering. **J.M. Grandner**, S. Yang, K.N. Houk

ORGN **540.** Synthesis of functionalized oligonucleotides of RNA using 2-methylbenzothiophenyl groups at the C2'-O- position of uridine and adenosine. **A.J. Francis**, M.J. Resendiz

ORGN **541.** Synthesis and evaluation of dye derivatives as G-quadruplex-stabilizing molecules. **J. McCallum**

ORGN **542.** Synthesis of β-APN derivatives for inhibition of the LOX enzyme. **R. Lottie**

ORGN **543.** Synthesis of menaquinone (MK) analogs and investigation into the solution structure of MK-1 and MK-1 (H_2). **J.T. Koehn**, B.J. Peters, C.N. Beuning, S.K. Dellinger, D.C. Crick, D.C. Crans

ORGN **544.** Reversibly photoactivatable Janelia Fluor dyes, and their utility in imaging cellular features beyond the diffraction limit. **F. Jradi**

ORGN **545.** Azaaurones: An unexplored scaffold for biological activity. **J.K. Noe**, S.T. Handy

ORGN **546.** Synthesis and analysis of propargylglycine-based derivatives as potential inhibitors of LpxC. **R. Roldan**, K. Wilson, M.L. Cafiero, L.W. Peterson

ORGN **547.** Fluorescent derivatives of arachidonic acid: Tools for studying the anti-cancer activity of prostaglandins. **J.L. Stanley**, R. Van Dross, W.E. Allen

ORGN **548.** Design, synthesis and biological effects of novel HDAC6 selective inhibitors. **A. Mahendran**, R. Breslow

ORGN **549.** Synthetic and metabolic studies of deuterium labeled drugs. B. Rawal, **K. Headrick**, R. Giron, J. Kim, M. Klosinski, S. Thomas, J. Lee, K.W. Jung

ORGN **550.** Comparative in vitro translation control using antisense γPNA. **C. Emanuelson**, T. Canady, B. Armitage

ORGN **551.** Novel architectures that exhibit potent and selective inhibition of protein tyrosine phosphatases implicated in cancers and metabolic disease. **K.A. Scott**, T. Shi, E. Chapman, J.T. Njardarson

ORGN **552.** Exploring vinylboronic acids as reactants in bioorthogonal chemistry. S. Eising, **K.M. Bonger**

ORGN **553.** Environment activable nanoprodrug: Two-step surveillance in the anticancer drug release. **S. Biswas**, J. Das, S. Barman, T. K. Maity, N. Singh

Section C

Moscone Center
Hall D

Chemistry of Fullerenes, Carbon Nanotubes & Graphene

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **554.** Rotation of benzofulvenes' exocyclic double bond and its effects on molecular conjugation. A. Glass, **J. Okubo**

ORGN **555.** Interaction of olefin metathesis and fullerenes. **A. Poater**

Section D

Moscone Center
Hall D

Materials, Devices & Switches

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **556.** Propeller-shaped molecular switches: Synthesis, solid-state structure, and photochemical properties. **D. Cameron**, S. Eisler

ORGN **557.** Synthesis and electronic properties of dibenzothieno-isoindole dione building blocks. **E. Albright**, S. Eisler

ORGN **558.** Building extended metal-organic frameworks from dimetal tetracarboxylate building units. **M. Strowbridge**, H. Abourahma

ORGN **559.** Crystal engineering of azobenzene cocrystals with non-linear optical properties. **E. Graff**, D. Curran, D.J. McGee, H. Abourahma

ORGN **560.** Changes in the intermolecular rotation of a crystalline carbazole rotor upon diffusion of volatile compounds. **A. Aguilar**, S. Perez Estrada, M. Rodríguez, B.V. Rodriguez-Molina

ORGN **561.** Phthalocyanine–chromophore dyads: Synthesis and photophysical studies. **R. Liu**, X. Zhang, D. Pockat, R. Moirangthem, J.S. Lindsey

ORGN **562.** Synthesis and characterization of asymmetric indenotetracenes: Novel n-type organic semiconductors for use in organic photovoltaics. **L. Purvis**, S. Ghosh, Z. Zhang, X. Gu, C.J. Douglas, C.J. Cramer, L. Gagliardi

ORGN **563.** Studies toward individual light-driven molecular motors. **H. Heideman**, M. Stoehr, B. Feringa

ORGN **564.** Withdrawn.

ORGN **565.** Exploration of *trans*-2-(1,2,3-triazolyl)-cyclohexanols as potential conformational switches. **M.R. Ruyonga**, V.V. Samoshin

ORGN **566.** Synthesis and electrochemical properties of functionalized iptycene-quinones. **Y. Ryu**, J. Kwon, K. Choi, B. An, S.Y. Park

ORGN **567.** Spin frustrated organic trisradical triangle. **Y. Wu**, M.D. Krzyaniak, M.R. Wasielewski

ORGN **568.** Red- and blue-shifted fluorescent polycyclic azaborine chromophores: Applications in organic materials. **J.A. Wilson**, L.L. Magill, R. Shavnore, C. McClinton, B. Brown, J. Vaughn, C.J. Saint-Louis, A. Schrock, M.T. Huggins

Section E

Moscone Center
Hall D

Molecular Recognition & Self-Assembly

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **569.** Synthesis of a water-soluble cubic porphyrin-based metallocomplex via click-chemistry. **A.R. Metell**, J.D. Thoburn

ORGN **570.** Synthetic steps toward a more soluble porphyrin-based M_8Por_6 metallocube. **M. Mitchler**, J.D. Thoburn

ORGN **571.** Pasteur's quasiracemates: A new look at an old story. **E.N. Pinter**, K.A. Wheeler

ORGN **572.** Molecular recognition boundaries of diarylamide quasiracemates. **I.C. Tinsley**, **B.L. Wagner**, K.A. Wheeler

ORGN **573.** Deconstructing crystal assemblies of 5-phenyl-1,3-dioxolan-4-ones using molecular shape. **K.A. Wheeler**, M.L. Grant

ORGN **574.** Tuning the optical properties of perylenemonoimide and the binding ability with cucurbit[8]uril via 9-position substitution. **L. Huang**, **G.H. Aryal**, K.W. Hunter

ORGN **575.** Strong fluorescent host-guest complexes based on cucurbit[8]uril and phenylalkyl quaternized perylenemonoimides. **G.H. Aryal**, **L. Huang**, K.W. Hunter

ORGN **576.** Separation of CO_2 from ambient air using a guanidine ligand. **C. Seipp**, N.J. Williams, M. Kidder, R. Custelcean

ORGN **577.** Self-assembly leads to recognition of divalent metal cation and tetrahedral divalent oxoanion using ditopic receptor. **S. Jansone-Popova**, A. Thevenet, R. Custelcean, B.A. Moyer

ORGN **578.** Synthesis of tetracyanoazulene as a guest for self-assembled Zn-porphyrin supramolecular cubes. **C.F. Ancajas**, J.D. Thoburn

ORGN **579.** Improved syntheses of tetraaminophenylporphyrin for use in supramolecular metallocubes. **P. Patel**, J.D. Thoburn

ORGN **580.** Using ^{19}F NMR spectroscopy to assess the strength of aromatic pi-pi interactions. **S.M. Strickland**, P. Li, K.D. Shimizu

ORGN **581.** Sensor of chirality and enantioselectivity for enantio-enriched molecules containing amines, alcohols, and carboxylic acids. **J. Zhang**, H. Gholami, M. Chun, B. Borhan

ORGN **582.** Self-folding multi-metal scaffold coordinator for hydrocarbon oxidation. **M. Mettry**

ORGN **583.** Synthesis of functionalized NHC-capped α-cyclodextrin metal complexes. **S.J. Bernardino**, M. Sollogoub

ORGN **584.** Graphene oxide-probe conjugate for the selective detection of pyrophosphate. **J.I. Hong**, D. Lee

ORGN **585.** Self-assembly of asymmetrically functionalized perylene diimide small molecules into well-defined structures. **R. Matthews**, J. Swisher, M. Tickerhoof, B. Rodier, E. Young, E. Pentzer

ORGN **586.** Ester-based synthetic information molecules. **F.T. Szczypinski**, C.A. Hunter

ORGN **587.** Synthesis and self-assembly of amphiphilic BINOLs in water. **F. Tosi**, J. Chen, B. Feringa

ORGN **588.** Synthesis of self-assembled bisrosette supramolecules. **c. Igci**, Y. Fan, A. Gonzales, K. Temburnikar, H. Fenniri, G.E. Gunbas

ORGN **589.** Synthesis and characterization of a new generation of molecular clips and their metal complexes. **M. Alaparthi**, A.G. Sykes

ORGN **590.** Supramolecular approaches to the protecting group chemistry. **V. Ramalingam**

ORGN **591.** New class of crown ether- verdazyl derivatives for sensing applications. D.J. Brook, **V. Balasubramanian**

ORGN **592.** Functionalized calixarenes: Synthesis, characterization and anion sensing applications. **N. Edwards**, F. Liu, D. Schnable

ORGN **593.** Controlling the conformations of molecules inside nano-space towards molecular protection and unique reactions in confined media. **K. Wang**, B.C. Gibb

Section F

Moscone Center
Hall D

Nanomaterials

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **594.** Synthesis of covalent organic frameworks for the upconversion of photons with nanocrystal light absorbers. **T.E. Dorado**, X. Li, M.L. Tang

ORGN **595.** Synthesis of calamitic mesogenic organic small molecules and their influence on the properties of CdSe/ZnS core–shell quantum dot nanocomposites. **G.I. Warren**, A. Keshavarz, S. Riahinasab, A. Elbaradei, L. Hirst, B.J. Stokes

ORGN **596.** Environmentally benign semifluorinated amphiphiles for drug delivery. **M. Fleetwood**, A. McCoy, S. Mecozzi

ORGN **597.** Withdrawn.

ORGN **598.** π-Conjugated polycyclic molecular systems and their supramolecular assemblies. **H. Sims**, H.P. Rathnayake

ORGN **599.** Withdrawn.

ORGN **600.** Evidence of splitting 1,2,3-triazole into alkyne and azide by low mechanical force in the presence of other covalent bonds. **A. Khanal**

ORGN **601.** New access to GNRs: Conversion of diarylpolydiacetylene polymers to graphene nanoribbons via mild heating. **R. Jordan**, R. Mccurdy, S. Khan, Y.F. Rubin

Section G

Moscone Center
Hall D

Peptides, Proteins & Amino Acids

S. M. Silverman, *Organizer*

5:30 - 7:30

ORGN **602.** Improving peptide purification via flash column chromatography by modulating mobile phase pH. **E. Denton**, J.R. Bickler

ORGN **603.** Proteolytic stabilization of β hairpins by α,β-dehydroamino acids. **K.G. Webber**, A. Jalan, S.L. Castle

ORGN **604.** Impact of peptide structure on proximity-driven reactivity with bifunctional helical catalysts. **B. Masino**

ORGN **605.** Detecting amyloid oligomer assembly in a chemical model system. **S. Yoo**, P.J. Salveson, A. Kreutzer, C.H. Hart, J.S. Nowick

ORGN **606.** X-ray crystallographic structures of a trimer, dodecamer, and annular pore formed by an $A\beta_{17-36}$ β-hairpin. **A. Kreutzer**, I.L. Hamza, R.K. Spencer, J.S. Nowick

ORGN **607.** Anion binding by N-protected fluorescent citrulline. **M. Muhammad**, W.E. Allen

ORGN **608.** Where the glow shouldn't go: Fluorescent arginine inside of membranes. **S. Marshall**, W.E. Allen

ORGN **609.** Excited-state properties of fluorescent arginine: Toward light-promoted cellular penetration. **M. DiVittorio**, W.E. Allen

ORGN **610.** Stabilizing the collagen triple helix with a ruthenium(II) anchor. **P. Banzon**, W.E. Allen

ORGN **611.** Silver(I)-promoted asparagine-based peptide ligation employing an *N*-terminal asparagine thioamide. **K. Shang**, C. Hutton

ORGN **612.** Structure activity relationship study of amino acid sulfonamide hydroxamic acid inhibitors for the botulinum neurotoxin LC. **S.L. Rodriquez-Beltran**, T.K. Lien, N.T. Salzameda

ORGN **613.** Design and synthesis of fibronectin-targeted peptide anticancer drug conjugates for targeted chemotherapy of prostate cancer. **S. Eun Park**, M. Bisoffi, K. Parang, R.K. Tiwari

ORGN **614.** New method for selective imide bond cleavage. **B. Island**, C. Hutton

ORGN **615.** Withdrawn.

ORGN **616.** Isolation, purification and partial characterization of *Crotalaria pallida* Ait seed proteins. **D. Bandyopadhyay**, S. Ukil, S. Laskar

ORGN **617.** Unusual amino acid from the seeds of *Abrus precatorius Linn.*: Isolation, characterization, *in silico and in vitro* anticancer evaluation. **D. Bandyopadhyay**, O. Espino, S. Laskar

ORGN **618.** Synthesis of cyclic peptide conjugate of curcumin and doxorubicin as a bidentate anticancer agent. **S. Darwish**, R.K. Tiwari, K. Parang

ORGN **619.** Substrate analogs for characterizing the substrate tolerance of *S. pneumoniae* sortase A. **O.G. Banks**, J. Antos

ORGN **620.** Contribution of bulky α, β - dehydroamino acids in the proteolytic stability of beta-hairpins. **A. Jalan**

ORGN **621.** Modification of human Hsp72 function by electrophilic compounds. **R.E. Connor**, A. Lieber

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

WEDNESDAY MORNING

Section A

Moscone Center
3018/3022

Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Junqi Li & Martin D. Burke

Cosponsored by WCC

K. B. Hansen, *Organizer*

A. Hill, *Organizer, Presiding*

9:00 ORGN **622.** Withdrawn.

9:45 ORGN **623.** Concepts and catalysts for anion-controlled organic synthesis. **D. Toste**

10:30 ORGN **624. Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry sponsored by Avantor™ Performance Materials). Natural productome project: Modularizing and generalizing natural product synthesis. **M.D. Burke**

11:15 ORGN **625. Award Address** (Nobel Laureate Signature Award for Graduate Education in Chemistry sponsored by Avantor™ Performance Materials). Automated small molecule synthesis via iterative coupling of boronate building blocks. **J. Li**, S.G. Ballmer, E. Gillis, S. Fujii, M.J. Schmidt, A. Palazzolo, J.W. Lehmann, G.F. Morehouse, M.D. Burke

Section B

Moscone Center
3014/3016

Chemical Biology: Enabling Drug Discovery

Cosponsored by BIOL

Financially supported by Celgene Corp.

R. E. Kyne, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 ORGN **626.** Translational chemical biology. **C.R. Bertozzi**

8:50 ORGN **627.** PROTACS: Induced protein degradation as a therapeutic strategy. **C.M. Crews**

9:35 ORGN **628.** Clickable photoaffinity probes to evaluate the selectivity of β-secretase inhibitors in live cells. **D.S. Johnson**

10:20 Intermission.

10:25 ORGN **629.** From serendipity to clinical trials: Discovery of reversible covalent kinase inhibitors. **J.W. Taunton**

11:10 ORGN **630.** Chemical-proteomic strategies to investigate reactive cysteines. **E. Weerapana**

11:55 Concluding Remarks.

Section C

Moscone Center
3011

Heterocycles & Aromatics

R. D. Broene, *Organizer*

J. R. Vyvyan, *Presiding*

8:00 ORGN **631.** Accessing chiral pyrrolines via an iron(III)-catalyzed carbonyl-olefin metathesis. **R. Harding**, E. Groso, A. Golonka, B. Alexander, C. Schindler

8:20 ORGN **632.** Hiyama couplings of oxasilacycloalkenes: Synthesis of trisubstituted Z-styrenes and application to natural product skeletons. **J.R. Vyvyan**, C.A. Engles, S.L. Bray, E.D. Wold, C.L. Porter, M.O. Konev

8:40 ORGN **633.** Harnessing cascade Suzuki-cyclization reactions of pyrazolo[3,4-*b*]pyridine for the synthesis of tetracyclic fused heteroaromatics. **F. Popowycz**, H. Lavrard

9:00 ORGN **634.** Polycyclic aromatic hydrocarbons via iron(III)-catalyzed carbonyl-olefin metathesis. **C. McAtee**, P. Riehl, C. Schindler

9:20 ORGN **635.** Diastereoselective synthesis of 2,4,6-trisubtituted piperdines via Prins cyclyization. **J.A. Hood**, M. Donahue

9:40 ORGN **636.** Alkylation, arylation, and cyclopropylation of common heterocycles via palladium catalysis. **J. Zhou**

10:00 ORGN **637.** Stereoselective synthesis of isoxazolidines *via* copper-catalyzed alkene diamination. **Z. Khoder**, C. Wong, S.R. Chemler

10:20 ORGN **638.** Redox controlled supramolecular chemistry based on viologen architectures. **J. Weiss**, J.A. Wytko, M. Berville

10:40 ORGN **639.** Withdrawn.

11:00 ORGN **640.** Photoluminescent phenalenyl-type radical. **O. Anamimoghadam**, **Y. Wu**, C. Pezzato, M.T. Nguyen, A. Samanta, S. Gozem, L. Mosca, A. Krylov, M.R. Wasielewski, F. Stoddart

11:20 ORGN **641.** Synthesis of biologically active marine natural rubrolides. **T.D. Silva**, M. Karak, J. Acosta, L.C. Barbosa, J. Boukouvalas

Section D

Moscone Center
3009

Molecular Recognition & Self-Assembly

R. D. Broene, *Organizer*

D. K. Smith, *Presiding*

8:00 ORGN **642.** Towards the characterization of the redox properties of shape-persistent macrocycles. **J. Dobscha**, C. Benson, Y. Liu, A.H. Flood

8:20 ORGN **643.** Logic-gated supramolecular disassembly and non-covalent guest release. **J. Gao**, X. Liu, H. Secinti, Z. Jiang, B. Zhao, Y. Xu, X. Guo, S. Thayumanavan

8:40 ORGN **644.** Stimuli-responsive self-assembly of organic cage compounds based on tribenzotriquinacenes. **A. Dhara**, F. Beuerle

9:00 ORGN **645.** Withdrawn.

9:20 ORGN **646.** General route to expanded helicenes. **G.R. Kiel**, T.D. Tilley

9:40 ORGN **647.** Cyclic voltammetry studies of a redox-responsive 4 H-bond ureidopyrimidinone alkyl-pyridinium capable of self-dimerization. **G. Darzi**, D.K. Smith

10:00 ORGN **648.** Synthesis and functional development of Calix[2]triazole[2]arene. **I. Kim**, J. Cho, S. Kim

10:20 ORGN **649.** Surface imprinted phosphopeptide capture beads. **C. Wierzbicka**, S. Torsetnes, O. Jensen, S. Shinde, B. Sellergren

10:40 ORGN **650.** Use of targeting motifs to improve oxidative catalytic breakdown of lignin in whole and fractionated biomass. **W.T. Hartwig**, J.J. Bozell

11:00 ORGN **651.** Colloidal and antibacterial studies of non-conventional polycationic amphiphiles. **K.L. Caran**, K. Seifert, K. Feitosa, J. Marafino, E. Rogers, K. Thompson, B. Walsh, S.D. Kendrick, K. McKenna, B. Ashamole, M.K. Lauer, S. Rauer, A. Rister

11:20 ORGN **652.** Redox-responsive dimerization in a ferrocene-containing four hydrogen-bond supramolecular assembly. **D.K. Smith**, M. Cedano

11:40 ORGN **653.** Design and synthesis of BODIPY based two-photo absorbing fluorescent dyes. **M. Shen**, X. Gao, X. He, N. Jian, J. Niu, X. Zhu, M. Song

Section E

Moscone Center
3007

Total Synthesis of Complex Molecules

R. D. Broene, *Organizer*

A. Angeles, *Presiding*

9:00 ORGN **654.** General strategy for the total synthesis of C-19 methyl substituted sarpagine/macroline indole alkaloids including macrocarpines A-G, peraksine, and dihydroperaksine. **M. Rahman**, J.R. Deschamps, J.M. Cook

9:20 ORGN **655.** Utilizing a C–C activation/cross-coupling strategy toward the total synthesis of taxagifine. **B.S. Wang**, B. Wyler, R. Sarpong

9:40 ORGN **656.** Studies toward the total synthesis of nagelamides A and C. **A.K. Herath**, M. Bhandari, C.J. Lovely

10:00 ORGN **657.** Application of phosphate tethers in polyketide synthesis: Efforts toward the synthesis of (*Z*)-cryptofolione and (+)-cryptocaryol A-D. **C.N. Ndi**, P.R. Hanson

10:20 ORGN **658.** Development of modular, pot-economical and library amenable strategies for the streamlined synthesis of bioactive natural products and analogs. **S. Javed**, M. Bodugam, A. Ganguly, G. Dissanayake, P.R. Hanson

10:40 ORGN **659.** Synthesis of the biselyngbyolides through rapid and convergent synthesis of C1–C13 fragment. **R.G. Thorat**, A.M. Harned

11:00 ORGN **660.** Enantioselective total synthesis of akuammiline alkaloids (+)-strictamine, (–)-2(*S*)-cathafoline, and (–)-aspidophylline A. **E. Picazo**, N.K. Garg

11:20 ORGN **661.** Concise synthesis of illudinine from dimedone. **A.E. Morrison**, G.B. Dudley

11:40 ORGN **662.** Flavin monooxygenase-mediated enantioselective oxidative dearomatization. **S. Dockrey**, A.R. Narayan

Section F

Moscone Center
3005

New Reactions & Methodology

R. D. Broene, *Organizer, Presiding*

8:00 ORGN **663.** Catalytic olefin dicarbofunctionalization. **R. Giri**

‡ *Cooperative Cosponsorship*

8:20 ORGN **664.** Novel application of Cu-Pd dual catalyst system for the cross-coupling of styryltrifluoroborates and amides. **M. Al-Masum**

8:40 ORGN **665.** Isothiourea-catalysed enantioselective formal [2+2] cycloaddition of perfluorinated alkyl-aryl ketones and homoanhydrides. **D. Barrios Antúnez**, A.D. Smith

9:00 ORGN **666.** Pd-catalyzed reactions of fluorinated enolates. **R.A. Altman**

9:20 ORGN **667.** Site-selective C(sp^3)-H activation enabled by *exo*-directing mode. **Y. Xu**, G. Dong

9:40 ORGN **668.** General platform for the selective methylene C(sp^3)–H activation of aliphatic amines. **A. Trowbridge**, K.F. Hogg, A. Álvarez Pérez, M. Gaunt

10:00 ORGN **669.** Small and uncommon diazoalkanes - applications in organic synthesis. **R.M. Koenigs**

10:20 ORGN **670.** Synthesis of azetidine derivatives *via* palladium-catalysed C(sp3)–H functionalisation of aliphatic secondary amines. **M. Nappi**, C. He, M. Gaunt

10:40 ORGN **671.** Ion pair-directed regiocontrol in transition-metal catalysis: A meta-selective C–H borylation of aromatic quaternary ammonium salts. **R. Phipps**, H.J. Davis, M.T. Mihai

11:00 ORGN **672.** Simple and efficient halogenation of C(sp^2)-H bonds directed by poorly coordinating functional groups: Scope and mechanistic investigation. **E. Erbing**, A. Sanz-Marco, A. Vázquez-Romero, J. Malmberg, M.J. Johansson, B. Martin-Matute

11:20 ORGN **673.** Discovery of a novel diastereoselective cuprate conjugate addition reaction and its application to the multi-kilogram synthesis of a clinical candidate. **S.W. Wright**, C. Choi, S. Chung, J.J. Mousseau, B.P. Boscoe, S.E. Drozda, J.D. Trzupek, K.L. Lee

11:40 ORGN **674.** Copper-catalyzed cyclization reaction for the synthesis of bicyclic α-carbonyl furan derivatives. **K. Hamal**, W. Chalifoux

WEDNESDAY AFTERNOON

Section A

Moscone Center
3018

Materials, Devices & Switches

R. D. Broene, *Organizer*

D. G. Patel, *Presiding*

1:00 ORGN **675.** Simple synthesis of complex molecular acceptors for high-performance air-processed and air-tested fullerene-free organic solar cells. **S.M. McAfee**, S. Dayneko, P. Josse, P. Blanchard, C. Cabanetos, G. Welch

1:20 ORGN **676.** Design and synthesis of phenothiazine based D-π-A chromophores exhibiting mechanofluorochromism and aggregation-induced emission. **T. Sachdeva**, S. Bishnoi, M.D. Milton

1:40 ORGN **677.** Self-healing molecular crystals. **P. Commins**, H. Hara, N. Pance

2:00 ORGN **678.** Movement of light-driven molecular motors on surfaces. **H. Heideman**, M. Stoehr, B. Feringa

2:20 ORGN **679.** Photomechanical molecular crystals based on anthracene derivatives. **F. Tong**, C.J. Bardeen, L. Zhu, R.O. Al-Kaysi, M.P. Hanson

2:40 ORGN **680.** Tuning charge carriers using electron deficient thiophenes. **J. Low**, B. Capozzi, J. Cui, S. Wei, L. Venkataraman, L. Campos

3:00 ORGN **681.** Development of selective and affordable small molecule sensors for an array of applications. **Y.J. Diaz**, Z.A. Page, A. Knight, N.J. Treat, J.R. Hemmer, C.J. Hawker, J. Read De Alaniz

3:20 ORGN **682.** Withdrawn.

3:40 ORGN **683.** Medium-dependent emission color of 2-(2-Hydroxyphenol) Benzoxazole (HBO) and click triazole derivatives. **Q.J. Meisner**, J.V. Accardo, L. Zhu

4:00 ORGN **684.** Redox active quinone based diarylethenes for light activated advanced materials. **D.G. Patel**

Section B

Moscone Center
3014

Peptides, Proteins & Amino Acids

R. D. Broene, *Organizer*

R. E. Moellering, *Presiding*

1:00 ORGN **685.** Facile method for the hydrolysis of a nickel Schiff-base complex. **C. Bontrager**, T. Geibel, G. Lengyel

1:20 ORGN **686.** Investigation of weak interactions using a β-hairpin peptide model system. **E.R. Danelius**, H. Andersson, P. Jarvoll, U. Brath, M. Erdelyi

1:40 ORGN **687.** Versatile, effective formation of biologically active single- and multi-loop peptide macrocycles via hydrazone condensation. **J.F. Reuther**, E.T. Hernandez, I. Kolesnichenko, E.V. Anslyn

2:00 ORGN **688.** Applying molecular dynamics simulations to engineer transaminase enzymes. **J.N. Sanders**, E.L. Noey, G. Jimenez-Oses, S. Osuna, K.N. Houk

2:20 ORGN **689.** Withdrawn.

2:40 ORGN **690.** Stabilization, assembly, and toxicity of trimers derived from Aβ. **A. Kreutzer**, S. Yoo, R.K. Spencer, J.S. Nowick

3:00 ORGN **691.** Withdrawn.

3:20 ORGN **692.** Introduction of o-(aminomethyl) phenyl-boronic acids into peptides: Alkylation of secondary amines. **E.T. Hernandez**, I. Kolesnichenko, J.F. Reuther, E.V. Anslyn

3:40 ORGN **693.** Efforts toward the synthesis of collision-induced dissociation-cleavable protein cross-linkers. **S. Block**, C. Yu, L. Huang, S.D. Rychnovsky

4:00 ORGN **694.** Stabilized α-helix-turn-3_{10}-helix inhibitors of RAB25 target context-specific phenotypes in cancer. **R.E. Moellering**

4:20 ORGN **695.** Triphenylmethane dyes that recognize oligomers of Aβ derived peptides. **P.J. Salveson**, A. Thuy-Boun, A. Kreutzer, S. Yoo, J.S. Nowick

Section C

Moscone Center
3011

Heterocycles & Aromatics

R. D. Broene, *Organizer*

J. J. Reczek, *Presiding*

1:00 ORGN **696.** In silico virtual and molecular docking screenings of pyrazole derivatives as estrogen antagonist. **L. Al-Tamimi**, A. Naqvi

1:20 ORGN **697.** Synthesis of 4,8-bis(2-dodecyloxy)benzo-[1,2-b:4,5-b] dithiophene-1,1,5,5-tetraoxide (BDTS) based organic semiconductors via copper-catalyzed C-H activation. **D. Khambhati**, T.L. Nelson

1:40 ORGN **698.** Synthesis of halogenated thiophenes, selenophenes, and benzo[*b*]selenophenes via environmentally benign halocyclization using sodium halides. **K. Giraudy**, J. Morgan, T. Kesharwani

2:00 ORGN **699.** Selective functionalization of pyridines and diazines via heterocyclic phosphonium salts. **A. McNally**, M. Hilton, R. Dolewski, L. Koniarczyk, X. Zhang, A. Overgard, J. Dowling

2:20 ORGN **700.** Synthesis, electrochemistry and antimicrobial properties of 1,2-benzisoxazole 2-oxides. **M.G. Kociolek**, K. Miller

2:40 ORGN **701.** Process development of GDC-0032 (Taselisib): Magnesium ethoxide promoted amidine formation and its application in fused imidazole synthesis. **D.R. Beaudry**, D.E. Carrera, S. Malhotra, R. Angelaud

3:00 ORGN **702.** Ferrocenyl chalcone salt derivatives: A study of their possible biological applications. **S.M. Delgado-Rivera**, G.E. Pérez-Ortiz, I. Montes-González, A.R. Guadalupe-Quiñones, D.J. Sanabria Ríos, A. Serrano-Brizuela, E. Colón-Lorenzo, A. Baerga-Ortiz, Y. Morales-Lozada

3:20 ORGN **703.** Radical chaperone-mediated directed C-H functionalization. **D.A. Nagib**

3:40 ORGN **704.** Efficient synthesis of highly-substituted anthraquinones. **J.J. Reczek**

4:00 ORGN **705.** OBO-methyl-ketone: A versatile pyruvate equivalent. **H. Esteves**, P. Smith, T.J. Donohoe

4:20 ORGN **706.** Heterocycle synthesis from quinols. **J. Wu**, S. Zheng

4:40 ORGN **707.** Catalytic Friedel-Crafts route into novel 3,3-diaryloxetane and dihydrobenzofuran motifs. **R.A. Croft**, J.J. Mousseau, C. Choi, J.A. Bull

Section D

Moscone Center
3009

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

R. D. Broene, *Organizer*

B. F. Gherman, *Presiding*

1:30 ORGN **708.** Dissociative electron-transfer reactions of polybrominated aliphatic electrophiles. **S.V. Rosokha**

1:50 ORGN **709.** Steric effects in the computational modeling of cyclization reactions of enyne-enones. K. Hoang, C.Q. Li, **B.F. Gherman**, J.D. Spence

2:10 ORGN **710.** Constructing a free-energy map for the initial steps of glycine: Glycolic acid co-oligomerization. **J. Kua**

2:30 ORGN **711.** Mechanistic insights on the transition-metal-catalyzed C-H amination reactions based on DFT studies. **X. Bao**

2:50 ORGN **712.** Photochemistry of crystalline 2-azidobiphenyls to form crystalline carbazoles: Scope, laser flash photolysis and solid-to-solid studies. **T. Chung**, M.A. Garcia-Garibay

3:10 ORGN **713.** Novel mechanism of molecular rotor fluorescence: Suppression of Kasha's rule. **M.E. Cousins**, H. Qian, I. Aprahamian, M.D. Liptak

3:30 ORGN **714.** Selective microwave heating of homogeneous organic reaction mixtures. **G.B. Dudley**, A.E. Stiegman

3:50 ORGN **715.** Using 19F and 1H NMR to determine the strength of intramolecular hydrogen bonds. **R.E. Rosenberg**

Section E

Moscone Center
3007

Total Synthesis of Complex Molecules

R. D. Broene, *Organizer*

T. G. Minehan, *Presiding*

1:30 ORGN **716.** Synthetic efforts toward the total synthesis of tubingensin B. **J. Kim**, N.K. Garg

1:50 ORGN **717.** Brocazine F: Studies towards total synthesis and divergence into screening library construction. A.I. Lansakara, W. Hulangamuwa, **R. Rafferty**

2:10 ORGN **718.** Late-stage strategies for the synthesis of ambiguine natural products. **R.E. Johnson**, M. Hartmann, L. Lang, S. Sawano, R. Sarpong

2:30 ORGN **719.** Synthesis of synoxazolidinone C. **N. Perry**, J.G. Pierce

2:50 ORGN **720.** Synthesis of complex molecules: Total synthesis and biological evaluation of Reniochalstatin E and analogs and synthetic work towards Laguanamide C. **A.J. Fatino**, C. Weese, G. Baca, A.I. Lansakara, R. Rafferty

3:10 ORGN **721.** Total synthesis of hortonones A-C. **T.G. Minehan**, H. Stambulyan

3:30 ORGN **722.** Studies toward a scalable second-generation total synthesis of the aplyronines as novel payloads for antibody-drug conjugates. **N. Anzicek**, S.R. Williams, M. Housden, I. Paterson

3:50 ORGN **723.** Enantioselective, convergent synthesis of the ineleganolide core by a tandem annulation cascade. J.L. Roizen, R.C. Smith, A.C. Jones, S. Virgil, B.M. Stoltz, **R. Craig**

4:10 ORGN **724.** Studies towards the total synthesis of Elisabethin A. **B. Schröder**, T. Gaich

Section F

Moscone Center
3005

New Reactions & Methodology

R. D. Broene, *Organizer*

G. Cuny, *Presiding*

1:00 ORGN **725.** Transition-metal-free synthesis of substituted aminocyclopropanes. **P. Cyr**, A. Côté-Raiche, S.M. Bronner

1:20 ORGN **726.** 1,2,3-Triazines: Powerful reagents for heterocycle synthesis. **C.M. Glinkerman**, D.L. Boger

1:40 ORGN **727.** Proton activated reactions of cyclopropylamine. **J.T. Ippoliti**, G.W. Larson

2:00 ORGN **728.** Asymmetric vinyolgous aza-Darzens approach towards the synthesis of vinyl aziridines. **P. Das**, I. Chogii, J.T. Njardarson

2:20 ORGN **729.** Lewis acid catalyzed carbonyl-olefin metathesis of aliphatic ketones. **H. Albright**, P. Riehl, C. McAtee, L. Karp, G. Rosenhauer, C. Schindler

2:40 ORGN **730.** *o*-Substituted anilines as a building block for the synthesis of aza heterocycles under transition-metal-free conditions. **G. Senadi**, J. Wang

3:00 ORGN **731.** Pyrimidine nucleosides with reactive β-keto sulfonyl group at C5 position. **S. Suzol**, A. Howlader, S.F. Wnuk

3:20 ORGN **732.** Development of a green and sustainable commercial manufacturing process for the antibiotic Zerbaxa™. **H. Ren**

3:40 ORGN **733.** One pot 1,3-amino alcohol synthesis *via* a hydrogen borrowing strategy. **R. Whittaker**

4:00 ORGN **734.** Acid-catalyzed cyclizations of α-hydroxymethyl cyclopropanes. **M. Sandridge**, S.A. France

4:20 ORGN **735.** Enantioselective heterodimerization of 1,3-dienes and acrylates. **S.M. Jing**, V. Balasanthiran, T. RajanBabu

WEDNESDAY EVENING

Section A

Moscone Center
West Hall

Heterocycles & Aromatics

S. M. Silverman, *Organizer*

7:00 - 9:00

ORGN **736.** Indole formation via palladium-catalyzed animation under mild pressure of 5% oxygen. **K.B. Clagg**, **S.G. Koenig**

ORGN **737.** Process optimization: Synthesis of a heterocyclic intermediate toward a RORc ligand. **J. Xu**, L.E. Sirois, R. Angelaud, D. Lao, F. Gosselin

ORGN **738.** Thermolysis reactions of phenylethylamino acid amides. **M. Casale**, D.A. Hunt

ORGN **739.** Base-mediated cyclization reaction of 2-(5-hydroxy-1-pentynyl) benzonitriles to 4-amino-2,3-dihydronaphtho[2,3-*b*]furanes and synthesis of furanonaphthoquinones. **M. Wu**

ORGN **740.** Synthesis of spirocyclic pyranoarenes via enal trapping of HDDA-generated benzynes. **C. Oswood**, T. Wang, T.R. Hoye

ORGN **741.** Building blocks for high temperature PEM fuel cells – Synthesis and characterization of crosslinking PAHs. **M. Zeyat**, D. Lentz

ORGN **742.** Intramolecular click reaction using carbocontiguous precursors. **F.A. Luzzio**, P.C. Patil

ORGN **743.** Atom-economical functionalization of pyrrole scaffolds: Synthesis of dihydropyrrolizines and tetrahydroindolizines enabled by titanocene(III) catalysis. **S. Hildebrandt**, A. Gansäuer

ORGN **744.** Thermal instability of 2,4 and 2,6-*N*-alkylamino disubstituted and 2-*N*-alkylamino substituted nitrobenzenes in weakly alkaline solution: Secamino effect. **D.K. Mohanty**, C. Walczak, A. Badour, C. Wade, M. Yonkey, T. Payne

ORGN **745.** Expedient access to highly functionalized iodoarylated allyic lactams: Application to the synthesis of macrocyclic enamidynes. **B. Mansker**, T. Beng

ORGN **746.** Modular access to potentially versatile 3-azaheterocyclic 1,5-enynes using cyclic α-chloro eneformamides. **S.A. Langevin**, T. Beng

ORGN **747.** Synthesis of 1-azaspiro[4.5] deca-1,3-dienes from N-propargylic β-enaminones. **E. Karadeniz**, M. Zora

ORGN **748.** Synthesis of propargyl-substituted pyrroles. **E.S. Yilmaz**, Y. Kelgokmen, M. Zora

ORGN **749.** Synthesis of heterocarbaporphyrins from carbatripyrrin intermediates. **T.J. Smolczyk**, T.D. Lash

ORGN **750.** Synthesis of azuliporphyrin dyads. **M. Metallo**, T.D. Lash

ORGN **751.** Synthesis and metalation of adj-dicarbaporphyrins. **W.T. Darrow**, T.D. Lash

ORGN **752.** Development of new routes for the synthesis of carbaporphyrins and carbachlorins. **N. Sahota**, T.D. Lash

ORGN **753.** Solubility switchable materials for printed organic electronics. **M. Ackermann**, J. Freudenberg, D. Jaensch, U. Bunz, K. Muellen

ORGN **754.** Finally an access to unsubstituted and structurally well-defined Poly-(Para-Phenylene) (PPP). **A. Abdulkarim**, F. Hinkel, D. Jaensch, J. Freudenberg, F. Golling, K. Muellen

ORGN **755.** Synthesis of heterocycles *via* transition metal catalyzed hydroarylation. **S. Acharya**, P. Zhao

ORGN **756.** Terephthalic acid analogs from celluloscic biomass. **E.M. Serum**

ORGN **757.** Synthesis of oxygen analogues of a promising anticancer drug. **F.M. Watts**, K.D. Berlin, D. Benbrook, R.A. Bunce

ORGN **758.** Bismuth(III) triflate catalyzed tandem esterification–Fries–oxa-Michael route to 4-chromanones. **R. Thing**, K. Meraz, K. Gnanasekaran, R.A. Bunce

ORGN **759.** Aromatic bromination in preference to addition to an alkene. **A.K. Giebink**, **D.E. Lewis**

ORGN **760.** Ultra-narrow low-landgap graphene nanoribbons from bromoperylenes: Synthesis and terahertz-spectroscopy. **D. Jaensch**, I. Ivanov, M. Baumgarten, M. Bonn, K. Muellen

ORGN **761.** Key improvements towards the preparation of antiretroviral drug tenofovir. **S. Korwar**, E. Yu, A.R. Ehle, J. Verghese, D. Rivalti, F. Gupton

ORGN **762.** Forgotten treasures: Synthesis and properties of *N*-substituted porphyrins. **S.S. Bernhard**, M. Roucan, M.O. Senge

ORGN **763.** Synthesis of oxetan-3-sulfides and sulfones as novel modules for medicinal chemistry. **R.A. Croft**, J.J. Mousseau, C. Choi, J.A. Bull

ORGN **764.** Withdrawn.

ORGN **765.** Synthesis and characterization of the synthon 1,2-di(4-pyrindinyl)ethan-1,2-dione dihydrochloride. **J.C. Martinez**, B. Coleman, R.J. Morgan, M.P. Castellani

ORGN **766.** Synthesis of novel fluorenofluorene-based structures. **A. Hacker**, M. Pavano, S. Genis, **D.K. Frantz**

ORGN **767.** NMR spectroscopic study of the identity and interconversion of conformers of 2-oxo-p-tert-butyltetramethoxycalix[4]arene. **J.L. Fantini**

ORGN **768.** Toward the templated synthesis of cyclophenylene structures comprising para- and meta-linkages. **E. Hajy**, M.B. Woodle, P.J. Sommerville, S.H. Vansdadia, Z.T. Sherman, K.R. Negri, R.R. Ponce, **D.K. Frantz**

ORGN **769.** Pyridinium zwitterion as a new dipole for the construction of heterocycles. **J. Lee**, D. Ko, J. Shim, J. Lee, E. Yoo

ORGN **770.** Effects of substituents on s-triazine reactivity. **S. Özcan**, A.E. Acar

ORGN **771.** HOF/CH_3CN: Excellent oxygen transfer agent for heterocycles. **S. Rozen**

ORGN **772.** Convenient synthesis of dihalo-substituted benzo[*b*] thiophenes *via* electrophilic cyclization. **A. Hayes**, **R. Romero**, C. Kornman, A. Tonnaer, T. Kesharwani

ORGN **773.** Approaches to synthesizing tetrahydrobenzazepine systems. **K. Dickson**, L.M. Bradley

ORGN **774.** Synthesis of novel exocyclic α,β-unsaturated dihydrolevoglucosenone derivatives via direct aldol condensation. **R. Hohol**, Z.J. Witczak, D.E. Mencer

ORGN **775.** Synthesis of chiral conformationally constrained diarylether cyclophanes. **B. Lindquist-Kleissler**, **D. Chadeayne**

ORGN **776.** Sterically overcrowded distyrylbenzenes: Tuning emission properties and photoreactivity. **J. Freudenberg**, F. Rominger, U. Bunz

ORGN **777.** Design, synthesis and characterization of novel thiazole based molecules. V. Patil, S.A. Patil, **S. Patil**

ORGN **778.** One-pot N-alkylation, ketonation and C-enolate alkylation of readily affordable γ-amido esters: Application to the synthesis of functionalized lactams. **J. Brooks**, T. Beng, E. O'Claire

ORGN **779.** Functionalized tetraazapentacenes as electron-transport materials. H. Reiss, T. Fritzensmeier, T. Marszalek, W. Pisula, P. Scharfer, U. Bunz, **F. Hinkel**

ORGN **780.** Reaction of oximes with 4-phenyl-1,2,4-triazoline-3,5-dione. **A.W. Jensen**, D.K. Mohanty, W.L. Dilling, D. Flotka, T. Xu, D. Saults

ORGN **781.** Tropone iron carbonyl complex as a platform for the synthesis of bridged nitrogen heterocycles. **D. Griffith**

ORGN **782.** Tuning the conformational equilibria in saturated heterocycles through the manipulation of a non-classical CH---O hydrogen bond: The importance of electrostatic interactions within small molecules. **K.M. Lambert**, W.F. Bailey, Z.D. Stempel, K.B. Wiberg, B.Q. Mercado

ORGN **783.** Synthesis of biphenyl and terphenyl precursor for π-conjugated Macrocyclic Molecular Belts (cMMBs). **T. Olson**, J. Lee, L. Fang

ORGN **784.** Intramolecular de Mayo photocyclization: The total synthesis of hippadine and pratosine. **C.I. Ochoa**, D.E. Minter, A. Haugen

ORGN **785.** Study of novel heterocycles for metal ion separation. **J. Shih**

ORGN **786.** Progress toward Au-catalyzed [4+1] cycloaddition of vicinally functionalized tertiary propargylic lactamoyl alcohols with diazoacetates. **M.S. Khim**, T. Beng

ORGN **787.** Azo dyes as ionochromic anion indicators. **S. McKee**, N.M. Paul

ORGN **788.** Improved method for the synthesis of 5,10,15,20-tetrakis (3,5-diacetamido-4-pyridyl)porphyrin. **S. Singh**

ORGN **789.** Parallel synthesis of aurones. **Z.E. Taylor**, S.T. Handy

ORGN **790.** First report of diastereodifferentiation of 2-azetidinones towards anticancer activity: Design, synthesis and *in vitro* evaluation. F. Olazarán-Santibáñez, **D. Bandyopadhyay**, P. Carranza-Rosales, G. Rivera, I. Balderas-Rentería

ORGN **791.** Microwave-assisted green synthesis of 1,3-thiazolidin-4-ones: An Insight. **D. Bandyopadhyay**, J. Strong

Section B

Moscone Center
West Hall

Flow Chemistry & Continuous Processes

S. M. Silverman, *Organizer*

7:00 - 9:00

ORGN **792.** Continuous processing approaches for prebiotic syntheses of 2-amino-oxazole and subsequent ribo/arabino furanosyl amino-oxazolines. **J. Kading**, A. Evans

ORGN **793.** Continuous bioprocessing/processing (enz-flow) approaches toward levomilnacipran synthesis. **M.G. Nguyen**, C. Ayoub, A.C. Evans

ORGN **794.** Towards a novel synthesis of levomilnacipran under continuous processing/bioprocessing conditions - reduction of the ester intermediate. **D. Sarmiento**, C. Ayoub, A. Evans

ORGN **795.** Effects of low gravity on chemical transformations. **A. Ku**

ORGN **796.** Multi-step continuous flow synthesis of diphenhydramine. **V. Vu**, D. Stout, J. Lim, G.W. Faris, J.P. Haushalter, J.P. Malerich, N. Collins

ORGN **797.** Multi-step continuous flow synthesis of fluconazole. **J. Szeto**, V. Vu, D. Stout, J. Lim, G.W. Faris, J.P. Haushalter, J.P. Malerich, N. Collins

ORGN **798.** Trans-hexenal preparation using microflow chemical system. **K. Wang**, L. Zhang, G. Luo

‡ *Cooperative Cosponsorship*

ORGN **799.** Synthesis of silylated diazo reagents via continuous flow synthesis. **C. Audubert**, O. Gamboa, H. Lebel

Section D

Moscone Center

West Hall

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

S. M. Silverman, *Organizer*

7:00 - 9:00

ORGN **800.** Fate of green fluorescent protein chromophore analogues with a positive charge at the phenyl-like group. J. Xu, Z. Zhang, R. Sung, **K. Sung**

ORGN **801.** Reactivity and dynamics of chlorocarbene additions to dibenzocyclooctyne. **A. Nadeem**, **A. Urquilla**, Y. Saperstein, V. Estes, A. Scorese, E. Dalchand, S. Tsuno, **D.C. Merrer**

ORGN **802.** Effect of chloro-stabilization on free radical halogenation. **A.J. LaPorte**, **M. Mielke**, J.A. Bjorklund, D.J. Rausch

ORGN **803.** Synthesis, photophysical and computational studies of a series of linear triazenes. **M.J. Voegtle**, K. Chikami, **R.A. Isovitsch**

ORGN **804.** Synthesis, pohtophysical, and computational studies of a series of 1,4-diaryl-1,3-butadiynes. **M. San Angelo**, **R.A. Isovitsch**

ORGN **805.** Intramolecular oxidative cyclization reactions of oximes and oxime ethers using alkenes as a potential nucleophiles or radical traps. **S. Baker**, N. Armada, E. Ho, A. Petit, P. De Lijser

ORGN **806.** Optimization and characterization of oxidative cyclization reactions of benzaldehyde oximes and oxime ethers with built-in heteroaromatic rings. **C. Taylor**, A. Alshreimi, P. De Lijser

ORGN **807.** Mechanistic aspects of the catalytic asymmetric allylboration of indoles and dihydroquinolines. **C. Diner**, M. Alam, S. Jonker, K. Szabo

ORGN **808.** Isolation and reactivity of trifluoromethyl iodonium salts. **J.N. Brantley**, A.V. Samant, D. Toste

ORGN **809.** Mechanistic investigation of Au(I)-phosphine catalyzed cycloisomerizations leads to a highly-selective novel Buchwald-type ligand. **A.H. Christian**, Z.L. Niemeyer, M.S. Sigman, D. Toste

ORGN **810.** Kinetic analysis of substituted tetraphenylacetones via Laser Flash Photolysis (LFP) in nanocrystalline suspensions. **J. Park**, M.A. Garcia-Garibay

ORGN **811.** Multiple oxidation pathways of photo-generated manganese(V)-oxo corroles. **N. Lee**, K. Kwong, D. Ranburger, R. Zhang

ORGN **812.** Computational study of heavy-atom tunneling in the Möbius π-bond shifting in [12]- and [16] annulene. **C.S. Michel**, **J.K. Arbitman**, I. Castano, W.L. Karney, C. Castro

ORGN **813.** Theoretical study of violapterin in gas phase and aqueous solution. **J.H. Kim**

ORGN **814.** Probing the effects of 1,3-cyclohexadiene substitution on the rates of retro-nitroso-Diels-Alder reactions. **J. Wong**, B.E. Lynde, **N.A. Yakelis**

ORGN **815.** *N*-substituted nitrosoguanidine Diels-Alder adducts: Synthesis and substituent effects on the rates of retro-Diels-Alder reactions. **M.N. Radford**, N.A. Yakelis

ORGN **816.** Hyperconjugative, secondary orbital, electrostatic, and steric effects on the reactivities and *endo* and *exo* stereoselectivities of cyclopropene Diels-Alder reactions. **B. Levandowski**, K.N. Houk

ORGN **817.** Computational studies on the mechanism of base-promoted rearrangement-cyclization of allylic esters. **P. Yu**, W. Li, K.N. Houk

ORGN **818.** Withdrawn.

ORGN **819.** Amide bond modulation: Cyclic amines and manipulating energy landscapes for conformational preferences using DEET analogs as a model system. J.G. Guerra, D. Manning, B. Mason, P. Kumar, B. Bajwa, S. Thompson, K. Maitra, K.V. Krishnan, **S. Maitra**

ORGN **820.** Computational elaboration of the mechanism of exocyclic ring formation of α,β-unsaturated carbonyls with guanine. **D.W. Boerth**, V.K. Sammeta, C. Paquin

ORGN **821.** Physical organic chemistry of phenylenevinylene systems for applications as MALDI matrices, photocatalyst and chemosensors. **C.A. Sierra**, J. Scaiano, C. Ochoa-Puentes, M.Y. Combariza, C. Blanco-Tirado

Section E

Moscone Center

West Hall

Total Synthesis of Complex Molecules

S. M. Silverman, *Organizer*

7:00 - 9:00

ORGN **822.** Recent progress toward the total synthesis of the arcutine family of natural products. **K. Owens**, Y. Hirooka, S. Ueno, R. Sarpong

ORGN **823.** Synthetic studies on guaipyridine alkaloids: Rupestines B-D and G. **S. Grosslight**, H. Spargo, P. Shelton, J.R. Vyvyan

ORGN **824.** Design and synthesis of archazolid-inspired V-ATPase inhibitors. **A.M. Craig**, G.W. O'Neil

ORGN **825.** Scalable copper mediated C-H hydroxylation: Synthesis of polyhydroxylated steroids. **Y. See**, A. Herrmann, R.A. Trammell, N. Xie, Y. Aihara, I. Garcia Bosch, P.S. Baran

ORGN **826.** Electrochemically promoted divergent synthesis of diterpene. **R. Merchant**, K.M. Oberg, A. Novak, P.S. Baran

ORGN **827.** Progress towards the total synthesis of himeradine A. **J. DeForest**, X. Li, S.D. Rychnovsky

ORGN **828.** Total synthesis of lycoricidine through chemical dearomatization of bromobenzene. **E.H. Southgate**, D.R. Holycross, D. Sarlah

ORGN **829.** Synthesis of antimalarial onocerane triterpene cupacinoxepin. M. Christmann, **F. Bartels**

ORGN **830.** Synthesis of desulfated 2-*epi*-symbioimine and related compounds via a highly stereoselective intramolecular Diels-Alder cycloaddition. **J.J. Chruma**, M. Xiang, Y. Wu, Z. Wang

ORGN **831.** Synthesis of beta-lactam analogs of the proteasome inhibitor belactosin A. N.K. Dunlap, **C. Harmon**

ORGN **832.** Synthesis of optically active crinine-type alkaloid precursors. **S.S. Bernhard**, N. Kümmerer, M.O. Senge, U. Nubbemeyer

ORGN **833.** Towards a total synthesis of cladosins E and G. **H.E. Burdge**, J. Mease, K.P. Reber

ORGN **834.** Synthetic studies towards the D ring of pectenotoxin-4. **M.S. Richardson**, C.J. Tame, T.J. Donohoe

ORGN **835.** Cyclization strategies for the total synthesis of biologically active natural products. **Z. Shultz**, J. Leahy

ORGN **836.** Towards the total synthesis and structural determination of patellazole B. **A. Phillips**, T. Balan, M. Anketell, S. Williams, I. Paterson

ORGN **837.** Withdrawn.

ORGN **838.** Progress towards the total synthesis of zamimaphidin A. **I. Hot**

ORGN **839.** Total synthesis of chaetoglobin A via asymmetric oxidative phenol coupling reaction. **H. Kang**, C. Torruellas, Y. Lee, M. Kozlowski

ORGN **840.** Towards molecular diversity with functionalized titanocenes. **E. Vogelsang**, A. Gansäuer

ORGN **841.** Progress toward the total synthesis of chrysophaentin A. **S. Jana**, K. Kim, C. Fullenkamp, C.A. Bewley, G.A. Sulikowski

ORGN **842.** Synthesis of 11-*cis*-retinol and its incorporation with FeO nanoparticle. **S. Lin**, J.D. Rainier

ORGN **843.** Total synthesis of taumycins A and B. **U.K. Shrestha**, T. Newar, J.N. deGruyter, W.A. Maio

ORGN **844.** Isocryptobeilic acid D: Synthetic pursuit and computational comparisons. **G.E. Miller**, **L. Kim**, **K.J. Kron**, **O. Velazquez**, **G.G. Castro**, R.J. Cave, D.A. Vosburg

ORGN **845.** Termination of cascade cyclizations by MOM-protected phenols. P. Shah, **D.F. Wiemer**

ORGN **846.** Concise synthesis of oncostemonols enabled by transition-metal catalyzed coupling reactions. **E.E. Sartor**, J. Cannon

ORGN **847.** Total synthesis of the α-alkylidene lactone natural products subamolides D and E. **K. Ng**, T.G. Minehan

ORGN **848.** Harnessing click reaction to synthesize mechanically interlocked cucurbit[n]uril molecules. **J. Partridge**, V. Ramalingam

ORGN **849.** Progress toward the total synthesis of Gymnastatin G. **J. Pham**, M.E. Jung, J. Ku

ORGN **850.** Synthesis and optical characterization of benzothiazole-curcumin derivatives for use in photodynamic therapy. **L. Howard**

ORGN **851.** Efforts in the development of new anticancer therapies: C-benzylated chalcones and derivatives. **J. Dallman**, A.I. Lansakara, T. Nguyen, R. Rafferty

ORGN **852.** Synthesis of four new englerin a analogs: Using enzimatic resolution to simplify synthetic pathways. **G. Bermudez**

ORGN **853.** Total synthesis of (+)-chimonanthine, (+)-folicanthine, (-)-calycanthine, and (+)-perophoramidine via solid state Norrish I photochemistry. **J. Dotson**, E. Rivera

THURSDAY MORNING

Section A

Moscone Center

3018

Materials, Devices & Switches

R. D. Broene, *Organizer*

D. J. Brook, *Presiding*

8:20 ORGN **854.** Redox active single-molecule switches. **X. Yin**, Y. Zang, L. Venkataraman, L. Campos

8:40 ORGN **855.** Synthesis, self assembly, and solar cell performance of N-annulated PDI small molecules. **A. Hendsbee**, G. Welch

9:00 ORGN **856.** Color-change photoswitching of an alkynylpyrene excimer dye. **R. Chan**

9:20 ORGN **857.** Novel oligo and polyacenes for intramolecular singlet fission devices. **A. Pun**, L. Campos

9:40 ORGN **858.** Towards simple low-cost molecular materials for use in air processed organic solar cells. **A. Payne**, S. Dayneko, G. Welch

10:00 ORGN **859.** Synthesis and assembly of discrete macrocycles related to two-dimensional covalent organic frameworks. **A.D. Chavez**, B.J. Smith, M.K. Smith, P. Beaucage, B.H. Northrop, W.R. Dichtel

10:20 ORGN **860.** Boron-containing conjugated materials with ultra-high Stokes shift. **J. Cassidy**, M. Bautista, I. Brettell-Adams, M. Smith, D.A. Dixon, P. Rupar, N. Hammer

10:40 ORGN **861.** Tunable highly fluorescent polycyclic azaborine chromophores: Applications in organic materials. **C.J. Saint-Louis**, M.T. Huggins, A. Schrock

11:00 ORGN **862.** Benzodithiophene (BDT) based small molecules for organic photovoltaics. **R. Gunawardhana**, C. Bulumulla, J. Du, M.C. Biewer, M.C. Stefan

11:20 ORGN **863.** Mixed valence in bis(verdazyl) systems. **D.J. Brook**

11:40 ORGN **864.** Withdrawn.

Section B

Moscone Center

3014

Chemistry of Nanomaterials, Fullerenes, Carbon Nanotubes & Graphene

Nanomaterials & Carbon Allotropes

R. D. Broene, *Organizer*

W. A. Braunecker, *Presiding*

8:00 ORGN **865.** Synthesis and photocatalytic activity of covalently conjugated three-dimensional pristine graphene–TiO_2 nanocomposite. **M. Yan**

8:20 ORGN **866.** Perfluoroalkylated fullerenes for stabilizing organic photovoltaic active layers. **W.A. Braunecker**, B.W. Larson, L.E. Garner, V.N. V., P.C. Ramamurthy, O.V. Boltalina, S.H. Strauss

8:40 ORGN **867.** Effects of structural features of graphene oxide on its tissue distribution in mice. **D. Jasim**, K. Kostarelos

9:00 ORGN **868.** Graphene nanoribbons through directed molecular assembly and stitching. R. Jordan, Y. Wang, R. Mccurdy, S. Khan, R.B. Kaner, **Y.F. Rubin**

9:20 ORGN **869.** Fabrication of supramolecular n/p- nanowires via coassembly of oppositely charged peptide-chromophore systems in aqueous media. **M. Khalily**, **B. Kucukoz**, **A. Karatay**, **G. Yaglioglu**, **M. Guler**

9:40 ORGN **870.** Withdrawn.

10:00 ORGN **871.** Perylene diimides as precise graphene-like mimetics of antioxidant carbon nanomaterials and of superoxide dismutase. **L.G. Nilewski**, A.S. Jalilov, V. Berka, C. Zhang, A. Yakovenko, G. Wu, T.A. Kent, A. Tsai, J.M. Tour

10:20 ORGN **872.** Synthesis of functionalized NHC-CO_2 adducts for applications in SERS-based sensing on noble metals. **J.F. DeJesus**, M.J. Trujillo, X. Gu, M.D. Stevens, J. Bradshaw, J.P. Camden, D.M. Jenkins

10:40 ORGN **873.** Clinically-translatable, targeted, polymeric nanoparticles for tissue accumulation. **N. Collins**, M.T. Proetto, N.C. Gianneschi

11:00 ORGN **874.** Cyclic peptide nanotubes with polar interior functionality. **S. Darnall**, C. Li, M. Alsina, S. Keten, B. Helms, T. Xu

11:20 ORGN **875.** Polymer-based retrograde nano-tracers as tools for neuroanatomy. **N. Zang**, T.B. Ditri, M. Tillo, D. Bortone, B. Bloodgood, M. Scanzain, N.C. Gianneschi

11:40 ORGN **876.** Scintillating possibilities of a drug assisted radiotherapy. **G.M. Entract**, R.W. Boyle

Section C

Moscone Center

3011

Flow Chemistry & Continuous Processes

R. D. Broene, *Organizer*

A. C. Evans, *Presiding*

8:30 ORGN **877.** Difluorodiazoethane: Applications in cycloaddition reactions. **L. Mertens**, K.J. Hock, R.M. Koenigs

8:50 ORGN **878.** Continuous bioprocessing (Enz-Flow) approaches toward levomilnacipran synthesis. **C. Ayoub**, M.G. Nguyen, A.C. Evans

9:10 ORGN **879.** *Trans*-cycloheptene, sila trans-cycloheptene and their application in bioorthogonal chemistry. **Y. Fang**

9:30 ORGN **880.** Arming THIOMAB Antibiotic Conjugates (TACs) through process chemistry. **S.G. Koenig**

9:50 ORGN **881.** Assessing inter- and intramolecular continuous-flow strategies towards methylphenidate hydrochloride. **R. Gérardy**, M. Winter, A. Vizza, J.M. Monbaliu

10:10 ORGN **882.** Catalyst-free thermal deprotection of tert-butyl esters. **S.J. Ryan**, K.P. Cole, R.D. Miller

10:30 ORGN **883.** AutoSyn: Toward a versatile multistep continuous synthesis device. **J.P. Malerich**, D. Stout, J.D. White, N. Collins

10:50 ORGN **884.** Flow chemistry with in-line analytics and feedback control. **M.G. Organ**

11:10 ORGN **885.** Continuous processing approaches for tunable asymmetric photochemical synthesis. **A.C. Evans**

Section D

Moscone Center

3009

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

R. D. Broene, *Organizer*

S. J. Sobeck, *Presiding*

8:30 ORGN **886.** Structure and photophysical property relationships of aminobenzoic acids. **S.J. Sobeck**, H. Rossiter

8:50 ORGN **887.** Photoremovable protecting group based on electrocyclic ring closure with leaving group expulsion via a putative zwitterionic intermediate. **G.N. Ndzeidze**, L. Li, M.G. Steinmetz

9:10 ORGN **888.** Hydrogen bonding directed photocatalytic hydrodefluorination, facile access to unsymmetric polyfluorinated aromatics. **M. Bani Khaled**, J.D. Weaver

9:30 ORGN **889.** Kinetic studies of various (trialkylsilyl)ethoxycarbonyl derivatives. **G.C. Daniels**, E. Camerino, J.H. Wynne, E.B. Iezzi

9:50 ORGN **890.** Mechanistic study of Cp^*Co^{III}/Rh^{III}-catalyzed directed C-H functionalization with diazo compounds. **S. Qu**, C.J. Cramer

10:10 ORGN **891.** N-hydroxyphthalimide (NHPI) mediated activation of C-H bonds with visible light using organic dyes. **S.S. Shah**, N.P. Singh

10:30 ORGN **892.** Synthesis and mechanistic exploration of novel P,N-ligated gold(I) compounds: Effect of pendant amine groups on catalytic enhancement. **J. Piedad**, A.C. Jones

10:50 ORGN **893.** Mechanistic evaluation of transition metal-catalyzed tetrahydroxydiboron-mediated H atom transfer from water. **T. Le**, S. Cummings, A. Brito, B.J. Stokes

11:10 ORGN **894.** Mechanism of Zn(II)/TMSCl-catalyzed hydroarylation. **S. Phan**, M. Desai, S. Wilkens, S. Patel, A. Villani-Gale, J. Devery

11:30 ORGN **895.** Photolysis of thiophene sulfonium ylides: Evidence for product sensitivity. **J. Kolattoor**, M.P. Sherman, W.S. Jenks

Section E

Moscone Center

3007

Total Synthesis of Complex Molecules

R. D. Broene, *Organizer*

Q. Dai, *Presiding*

8:30 ORGN **896.** Harnessing persistent radicals and stable quinone methide intermediates for the synthesis of resveratrol oligomers. **K.J. Romero**, X. Zhu, C. Stephenson

8:50 ORGN **897.** Enantioselective syntheses of rearranged abietane diterpenoids isolated from *Tripterygium wilfordii*. **R. Ali**, T.W. Bell

9:10 ORGN **898.** Synthetic efforts towards mandelalide/madeirolide A hybrid structures. **J. Li**, A. Ghosh, N. Veerasamy, R.G. Carter

9:30 ORGN **899.** Studies directed toward the synthesis of aspidophytine. **Y.E. Turkmen**, M. Gravel, V.H. Rawal

9:50 ORGN **900.** Catalyst-controlled oligomerization for the synthesis of polypyrroloindoline natural products. **J.J. Badillo**, C.R. Jamison, J. Lipshultz, R.J. Comito, D.W. MacMillan

10:10 ORGN **901.** Total synthesis of clerobungin A. **K.P. Reber**, J. Mease

10:30 ORGN **902.** Synthetic studies towards fischerindoles and ambiguines. **J. Xu**, V.H. Rawal

10:50 ORGN **903.** Studies towards the total synthesis of nahuoic acids. **Q. Liu**, Y. Deng, A.B. Smith, III

11:10 ORGN **904.** Exploration of gold(I)-catalyzed alkoxylation for formal synthesis of (+)-laurencin. **H. Park**, M. Lanier, P. Mukherjee, A.A. Ribeiro, R. Widenhoefer, J. Hong

11:30 ORGN **905.** Development and kilogram-scale synthesis of GSK2132838A. **Q. Dai**

Section F

Moscone Center

3005

New Reactions & Methodology

R. D. Broene, *Organizer*

D. R. Stuart, *Presiding*

8:00 ORGN **906.** Towards effective catalytic $C_2 + N_1$ aziridination with organic azides for organic synthesis. P.P. Chandrachud, L.C. Keller, J. Kern, G. Elpitiya, S. Roy, **D.M. Jenkins**

8:20 ORGN **907.** Synthesis of heterocyclic aldehydes and lactams involving aerobic copper-catalyzed alkene aminooxygenation. **T. Wdowik**, S.R. Chemler

8:40 ORGN **908.** Second generation oxirane-based approach for polypropionate construction: Application to the synthesis of ansamycins. **J.A. Prieto**, W. Torres, D. Rodriguez-Reyes, A. Cruz-Montanez

9:00 ORGN **909.** Hypervalent iodine(III)-promoted N-incorporation into N-aryl vinylogous carbamates to quinoxaline diesters: Access to 1, 4, 5, 8 tetraazaphenanthrene. **S. Arepally**, S.S. Duddu

9:20 ORGN **910.** Metal-free arylation reactions with unsymmetrical diaryliodonium salts. **D.R. Stuart**

9:40 ORGN **911.** Synthesis of enantiomerically pure 6-substituted-piperazine-2-acetic acid esters for Fragment Based Lead Discovery (FBLD). **S. Chamakuri**

10:00 ORGN **912.** Regio- and stereoselective oxyamination of dienes via tandem aziridination/ring-opening of dienyl carbamates. **S. Castillon**, I. Gimenez, J. Guasch, Y. Diaz, I. Matheu

10:20 ORGN **913.** Solvent- and catalyst-free, quantitative protection of hydroxyl, thiol, carboxylic acid, amide and heterocyclic amino functional groups. **B. Ahmed**, M.L. Jawor, G. Mezei

10:40 ORGN **914.** Bio-based amines and amides from renewable isosorbide. **F. Popowycz**, M. Janvier, S. Moebs-Sanchez

11:00 ORGN **915.** Withdrawn.

11:20 ORGN **916.** Mechanism-based solution to the ProTide synthesis problem. **S.M. Silverman**, B. Simmons, Z. Liu, A. Klapars, A. Bellomo

11:40 ORGN **917.** Flexible route to bioactive 6-alkyl-α-pyrones. **Y. Qu**, G.A. Kraus

THURSDAY AFTERNOON

Section A

Moscone Center

3009

Advanced Materials Technologies, Systems & Processes

R. D. Broene, *Organizer*

A. R. Lippert, *Presiding*

1:00 ORGN **918.** Single-molecule peptide sequecing: Side chain modification and model peptide sequencing studies. **E.T. Hernandez**, J. Swaminathan, A. Boulgakov, A. Bardo, L. Bachman, A. Johnson

1:20 ORGN **919.** Thio-amine click and declick reactions. **I. Kolesnichenko**, K. Diehl, S. Robotham, J. Brodbelt, E.V. Anslyn

1:40 ORGN **920.** Advanced photoswitch displays for volumetric 3D image generation. **A.R. Lippert**

2:00 ORGN **921.** Synthesis of a novel photoreactive collagen-like peptide and its one and two-photon absorption properties. **A. Ornelas**, K.N. Williams, K.A. Hatch, A. Paez, T. Boland, C. Li, K. Michael

2:20 ORGN **922.** Synthesis of (7*R*,8a*S*)-octahydro-5,5-dimethylindolizin-7-amine and (7S,8aS)-octahydro-5,5-dimethylindolizin-7-ol using an enzymatic resolution approach. **R.S. Kolluri**

2:40 ORGN **923.** Synthesis and biological evaluation of α-methoxylated acetylenic fatty acids. **C. Morales Guzman**, E. Álvarez Benedicto, Z. Torres Martinez, Y. Delgado Reyes, D.J. Sanabria Ríos, A.D. Tinoco, R. Balaña Fauce, N.M. Carballeira

3:00 ORGN **924.** One-pot electrocatalytic oxidation/photocatalytic C–O bond cleavage of lignin systems at ambient temperature. **I. Bosque Martínez**, C. Stephenson

3:20 ORGN **925.** Linking substance mixture information with physical properties for discovery. **P. Son**, V.A. Biehl, E.M. Altizer, A. Windhof, R.B. McWhirter

3:40 ORGN **926.** Controlling antimicrobial agents' release: Natural polymer-based encapsulation systems. **R. Rutenberg**, E. Poverenov, E. Fallik

Section B

Moscone Center

3011

Physical Organic Chemistry: Calculations, Mechanisms, Photochemistry & High-Energy Species

R. D. Broene, *Organizer*

D. A. Vosburg, *Presiding*

1:00 ORGN **927.** Mechanistic complexities of catalytic dihydropyridine reactions. **C. Hanson**, H. Vonesh, M. Solans, A. Nudo, S. Chowdhury, E. Kaydanovsky, J. Devery

‡ *Cooperative Cosponsorship*

1:20 ORGN **928.** How cinchona alkaloids steer the product distribution in the reactions of oxindoles with nitrosobenzene. **N. Celebi-Olcum**

1:40 ORGN **929.** N-heterocyclic carbene catalyzed ring opening polymerization of glycolide and lactide: A theoretical study. **X. Dong**, Y. Li, J.M. Grandner, K.N. Houk

2:00 ORGN **930.** Alkyne metathesis to delineate the effect of building block size on organic cage synthesis. **A. Yang**, J.S. Moore

2:20 ORGN **931.** Conjugated trimeric scaffolds accessible using indolyne cyclotrimerizations. **J. Lin**, T. Shah, A. Goetz, K.N. Houk, N.K. Garg

2:40 ORGN **932.** Non-bonding S–O interactions: A new element of stereocontrol and catalysis? **D. Walden**, E. Robinson, T. West, C. Fallan, J. Taylor, M. Greenhalgh, A.D. Smith, P. Ha-Yeon Cheong

3:00 ORGN **933.** Withdrawn.

3:20 ORGN **934.** Computational exploration of copper catalyzed azide-alkyne coupling reactions. **S. Bidwell**, H.P. Hratchian

3:40 ORGN **935.** Computational comparisons of Diels-Alder transition states for endiandric tetracycles using density functional theory. K.J. Kron, R.J. Cave, **D.A. Vosburg**

PHYS

Division of Physical Chemistry

J. Shea, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Elucidation of Mechanisms & Kinetics on Surfaces (see *CATL*, Sun, Mon, Tue, Wed, Thu)

Light-Driven Chemistry: Photoelectrochemistry & Photocatalysis (see *CATL*, Mon, Tue, Wed)

Nanoscience & Nanotechnology for Advanced Materials & Technologies (see *MPPG*, Mon)

Nanoscale Spectroscopic Characterization of Catalysts & Polymers (see *PMSE*, Sun, Mon)

SUNDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Cosponsored by INOR

S. Corcelli, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 PHYS **1.** Scanning tunneling microscopy of alkyl-substituted oligothiophenes on Au(111): Real-space visualization of molecular electronic structure. **B. Taber**, G. Nazin

8:50 PHYS **2.** Mixed-valence molecules: Direct imaging of intramolecular charge distribution by STM. **S. Kandel**

9:30 Intermission.

9:50 PHYS **3.** Spin effects on photo-induced electron and energy transfer processes in polynuclear donor-acceptor assemblies. **J.K. McCusker**

10:30 PHYS **4.** Energy transfer in quantum dot-molecule assemblies. **E.A. Weiss**, C. Wang, K. Lee, M. Kodaimati, S. Homan, G.C. Schatz

11:10 PHYS **5.** Nanocrystal taxonomy and ligand alphabet soup: Covalent bond classification system applied to surface chemistry. **N.C. Anderson**, N.R. Neale, J.S. Owen

Section B

Parc 55 San Francisco

Mason

Long Range Correlated Motions in Proteins

Protein Dynamics & Allostery

A. Markelz, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 PHYS **6.** Mind the gap: Building a bridge between physical and statistical models of allostery. M.A. Cuendet, G. Khelashvili, H. Weinstein, **M.V. LeVine**

9:35 PHYS **7.** Entropy in protein function. **A.J. Wand**

10:05 PHYS **8.** Predicting optimal allosteric stabilization sites with contact stabilization analysis. **A. Dickson**, C. Bailey, J. Karanicolas

10:25 Intermission.

10:40 PHYS **9.** Allosteric dynamics of AMPA receptors and coupling to membrane fluctuations. J. Lee, J. Krieger, I. Greger, **I. Bahar**

11:10 PHYS **10.** Understanding allosteric regulation of G protein-coupled receptors using molecular simulation. **A. Grossfield**

11:40 PHYS **11.** Opening of the intracellular gate affects the structure and ion occupancy of the selectivity filter of a potassium ion channel. **H.T. Kratochvil**, M.T. Zanni

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photosynthesis

K. Glusac, M. Olivucci, *Organizers*

D. S. Larsen, *Organizer, Presiding*

8:00 PHYS **12.** Probing ultrafast dynamics of photosynthetic reaction centers using two-dimensional electronic spectroscopy. **J.P. Ogilvie**, V. Policht, A. Niedringhaus, A. Loukianov

8:30 PHYS **13.** Structural and functional modularity of the orange carotenoid protein in governing cyanobacterial photoprotection. **C. Kerfeld**

9:00 PHYS **14.** Biomimetic designs and *In-Situ* x-ray structural characterization of catalysts for the artificial leaf. **D.M. Tiede**, G. Kwon, I. Kim, J. Emery, A.B. Martinson

9:30 PHYS **15.** Photophysics of coupled carotenoids. **M.J. Tauber**

10:00 Intermission.

10:20 PHYS **16.** Photochemical water oxidation by photosystem II. **G.W. Brudvig**

10:50 PHYS **17.** Pyridine Co-catalysis impacting CO_2 reduction over semiconductor photoelectrodes. **T. Senftle**, E.A. Carter

11:20 PHYS **18.** Energy transfer mechanisms in green sulphur bacteria. **D. Zigmantas**, J. Dostal, K. Zidek, K. Kim, M. Alcocer, D. Bina, H. Lokstein, J. Psencik

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Simulating Electrons on Large Scale

Cosponsored by COMP

O. V. Prezhdo, *Organizer*

A. V. Akimov, *Organizer, Presiding*

8:00 PHYS **19.** Spectroscopy of molecules at metal surfaces: Markovian and non-Markovian electron dynamics. **M. Pavanello**

8:40 PHYS **20.** Patches for realtime TDDFT: Correlation and a time-dependent Tamm-Dancoff approximation. **J. Parkhill**

9:20 Intermission.

9:35 PHYS **21.** Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states. M.G. Bayne, **A. Chakraborty**

10:15 PHYS **22.** Spectra from stochastic many-body methods. **V. Vlcek**, R. Baer, E. Rabani, D. Neuhauser

10:35 PHYS **23.** Description of quasiparticles in stochastic many-body methods. V. Vlcek, R. Baer, E. Rabani, **D. Neuhauser**

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Ahmed Zewail Award in Ultrafast Science & Technology: Symposium in honor of Stephen R. Leone

Cosponsored by PRES

J. E. Shea, *Organizer*

D. Zhong, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **24.** From ultrafast spectroscopy to structural dynamics. **M. Chergui**

8:45 PHYS **25.** In search of transition states of chemical reactions. A tribute to Ahmed Zewail. **L. Banares**

9:25 Intermission.

9:40 PHYS **26. Award Address** (Ahmed Zewail Award in Ultrafast Science & Technology sponsored by the Ahmed Zewail Endowment Fund by the Newport Corporation (Newport)). Ultrafast x-ray dynamics. **S.R. Leone**

10:40 PHYS **27.** Probed quantum systems from the inside: On the attosecond time scale. **P. Corkum**

11:20 PHYS **28.** Anion photoelectron/photodissociation spectroscopies: Ozonide solvation dynamics. **W.C. Lineberger**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Interfaces

A. T. Krummel, N. E. Levinger, *Organizers*

K. Gaffney, *Presiding*

8:00 Introductory Remarks.

8:20 PHYS **29.** Is the surface of clathrate hydrates hydrophilic or oleophilic? **V. Molinero**

9:00 PHYS **30.** Solvation and confinement effects on the thermodynamics of helix coil transitions of polyalanine in open nanotubes. D. Suvlu, S. Samaratunga, D. Thirumalai, **J.C. Rasaiah**

9:20 PHYS **31.** Ion-induced stabilization of palmitic acid monolayers. **H.C. Allen**, E. Adams, B. Wellen, A. Vidalis, T. Zhang

10:00 Intermission.

10:20 PHYS **32.** Quantitative prediction of position and orientation for a polyhedral nanoparticle at liquid/liquid interfaces. **S. Li**

11:00 PHYS **33.** Asymmetric electrowetting at the nanoscale: Molecular dynamics simulations of molecular fluids on graphene. **N. van der Vegt**

11:20 PHYS **34.** Rate theory on ion pairings at the liquid/vapor interface of water. **L.X. Dang**

Advanced X-Ray Techniques for Catalyst Characterization

Catalysts in Action

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Allosteric Regulation & Mechanisms

Sponsored by COMP, Cosponsored by PHYS

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

Coherent Multidimensional Spectroscopy in Materials Science

Sponsored by ANYL, Cosponsored by PHYS

SUNDAY AFTERNOON

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Theory & Modeling

Cosponsored by INOR

S. Corcelli, *Organizer*

S. Kandel, *Presiding*

1:30 PHYS **35.** Charge motion in disordered molecular solids. **M.A. Ratner**

2:10 PHYS **36.** Electronically excited states of organic molecules and transition-metal containing systems are a challenge for quantum chemistry. **L. Gagliardi**

2:50 Intermission.

3:10 PHYS **37.** Theoretical studies of homogeneous and heterogeneous multicenter electrocatalysts. **S. Hammes-Schiffer**

3:50 PHYS **38.** Spectroscopy and electron transfer processes in molecular systems of multi metal centers: Insight by *ab-initio* modeling. **B.D. Dunietz**

4:30 PHYS **39.** Efficient implementation and assessment of open-shell symmetry-adapted perturbation theory. **J.F. Gonthier**, L. Dos Anjos Cunha, C.D. Sherrill

Section B

Parc 55 San Francisco

Mason

Long Range Correlated Motions in Proteins

Protein-Solvent Modeling: Refinement through Comparison with Measurements

A. Markelz, *Organizer*

A. J. Wand, *Presiding*

1:30 PHYS **40.** Spectral analysis of correlated protein and protein-water vibrations in molecular dynamic simulations. **M. Heyden**

2:00 PHYS **41.** 2D-Raman-THz spectroscopy of water and aqueous salt solutions. A. Shalit, D. Sidler, **P. Hamm**

2:30 PHYS **42.** Correlated vibrational motion in the Fenna-Matthews-Olson complex. **B.S. Rolczynski**, H. Zheng, V.P. Singh, P. Navotnaya, J.R. Caram, K. Ashraf, A.T. Gardiner, R.J. Cogdell, G.S. Engel

2:50 PHYS **43.** Protein intramolecular vibrations couple to the dynamical transition. **M. Xu**, K. Niessen, Y. Deng, N. Michki, A. Markelz

3:10 PHYS **44.** Towards development of the *ab-initio*-based force field for biological systems. **P. Gurunathan**, L.V. Slipchenko

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photochemistry & Emerging Techniques

K. Glusac, M. Olivucci, *Organizers*

D. S. Larsen, *Organizer, Presiding*

1:30 PHYS **45.** Controlling the photostability of uracil with shaped light fields. D. Keefer, S. Thallmair, S. Matsika, **R. de Vivie-Riedle**

2:00 PHYS **46.** Using fundamental photochemistry to drive drug development and structural-biology applications. **C.E. Crespo-Hernandez**

2:30 PHYS **47.** Direct evidence of molecular charge accumulation during solar excitation of molecular dyes, and guidelines for obtaining large quantum yields. H. Chen, J.M. Cardon, **S. Ardo**

2:50 PHYS **48.** Operating photoswitches with sunlight. **S. Hecht PhD**

3:20 PHYS **49.** Fuel from water: The reductive side of water splitting and the light-driven generation of hydrogen. **R. Eisenberg**, H. Lv

3:50 Intermission.

4:10 PHYS **50.** Photochemical pathways for motion in E/Z photoswitchable thienyl-ethenes. **A.E. Bragg**

4:40 PHYS **51.** Combined experimental and theoretical study of the transient IR spectroscopy of 7-hydroxyquinoline in the first electronically excited singlet state. F. Hoffmann, M. Ekimova, G. Bekçioğlu-Neff, **E. Nibbering**, D. Sebastiani

5:00 PHYS **52.** Subensemble-Selective photochemistry by mixed IR/VIS two-dimensional spectroscopy. **J. Bredenbeck**

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Simulating Quantum Nuclei on Large Scale

Cosponsored by COMP

O. V. Prezhdo, *Organizer*

A. V. Akimov, *Organizer, Presiding*

1:30 PHYS **53.** Linearized path integral methods for capturing quantum effects in molecular dynamics simulations of condensed phase systems. **E. Geva**

2:10 PHYS **54.** Phase space vs. coordinate space approaches for overcoming exponential scaling in large quantum calculations. H. Larsson, B. Hartke, **D. Tannor**

2:50 PHYS **55.** Path integral methods for nonadiabatic dynamics: Quantum transitions from classical trajectories. **N. Ananth**

3:30 Intermission.

3:45 PHYS **56.** Molecular dynamics of large systems with quantum corrections for selected nuclei. **S. Garashchuk**

4:25 PHYS **57.** Nonadiabatic molecular dynamics with time-domain density functional theory. **O.V. Prezhdo**

5:05 PHYS **58.** Condensed phase non-adiabatic dynamics from temporally-interpolated memory kernels. **D. Hait**, M. Mavros, T.A. Van Voorhis

5:25 PHYS **59.** Preparation of a single highly vibrationally excited quantum state using Stark induced adiabatic Raman passage. **W. Perreault**, N. Mukherjee, R.N. Zare

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Ahmed Zewail Award in Ultrafast Science & Technology: Symposium in Honor of Stephen R. Leone

Cosponsored by PRES

J. E. Shea, *Organizer*

S. R. Leone, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS **60.** Ultrafast protein folding. **M. Gruebele**

2:10 PHYS **61.** How to turn a right hand into left: Chiral plasmons and more. **V.A. Apkarian**

2:45 PHYS **62.** Probing and controlling molecular electronic and vibrational states with shaped laser pulses. **M. Dantus**

3:20 Intermission.

3:35 PHYS **63.** Probing ultrafast photochemical processes in solution with femtosecond spectroscopies. **M.H. Khalil**

4:10 PHYS **64.** Better chemical filters for better life. **V. Stavros**, N.C. Cole-Filipiak, M. Staniforth, M. Horbury, N.D. Rodrigues, L.A. Baker, J. Woolley

4:45 PHYS **65.** Dynamics and mechanism of ultrafast water-protein interactions. **D. Zhong**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Liquids

A. T. Krummel, N. E. Levinger, *Organizers*

W. H. Thompson, *Presiding*

1:30 PHYS **66.** Measuring liquid density using optical Kerr effect spectroscopy. J.S. Bender, S. Cohen, X. He, B. Coasne, **J.T. Fourkas**

2:10 PHYS **67.** Combined FT-IR and soft-x-ray spectroscopic approach on aqueous ammonium and ammonia. M. Ekimova, W. Quevedo, L. Szyc, P. Wernet, M. Odelius, **E. Nibbering**

2:30 PHYS **68.** Structure and dynamics of glyme based electrolytes for sodium based rechargeable batteries. **R. Kumar**, R. Jorn, D.G. Kuroda

3:10 Intermission.

3:30 PHYS **69.** Ultrafast x-ray scattering studies of solvent and solvation dynamics. **K. Gaffney**, T.B. van Driel, K. Kjaer, R. Hartsock, A. Dohn, K. Moller, M. Nielsen, T. Harlang

4:10 PHYS **70.** Dramatic impact of confinement on sugars and carbohydrates in confined environments. **N.E. Levinger**, B.P. Wiebenga-Sanford

4:30 PHYS **71.** Solvation dynamics of hydrated electrons: Connecting hydrated electron structure to time-resolved photoelectron spectroscopy and temperature-dependent transient absorption experiments. **B.J. Schwartz**, C. Zho, E. Farr, W.J. Glover

Advanced X-Ray Techniques for Catalyst Characterization

Theory & Beyond

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LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Synthesis & Characterization of Materials for Energy Applications

In Operando & Surface Sensitive Analysis

Sponsored by ANYL, Cosponsored by PHYS

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

Coherent Multidimensional Spectroscopy in Materials Science

Sponsored by ANYL, Cosponsored by PHYS

MONDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Cosponsored by INOR

S. Corcelli, *Organizer*

L. J. Webb, *Presiding*

8:00 PHYS **72.** Electrical transport in MOFs. **M. Dinca**, L. Sun, S. Park, G. Skorupskii, L. Xie, C. Hendon

8:40 PHYS **73.** Solar photochemistry of semiconductor nanocrystals coupled with redox catalysts. **G. Dukovic**

9:20 PHYS **74.** Charge transfer between hydrogen-bonded metal-metal quadruple bonds. L. Brown, A.J. Meijer, **N. Patmore**, K.B. Vincent, L. Wilkinson

10:00 Intermission.

10:20 PHYS **75.** Mixed-valency across hydrogen bonds: The effects of electron delocalization. **C.P. Kubiak**, T.M. Porter

‡ *Cooperative Cosponsorship*

11:00 PHYS **76.** Role of molecular assemblies in dye sensitized photoelectrosynthesis cells. **T.J. Meyer**, L. Alibabaei, M.K. Brennaman, B. Sherman, D. Wang, M. Eberhart, M. Sheridan, A. Nayak, Y. Wang

11:40 PHYS **77.** Synthesis and characterization of exactly doped semiconductor quantum dots. **A. Hassan**

Section B

Parc 55 San Francisco

Powell

Long Range Correlated Motions in Proteins

Measurement Techniques

A. Markelz, *Organizer*

M. Heyden, *Presiding*

9:00 PHYS **78. Award Address** (Nakanishi Prize sponsored by the Nakanishi Prize Endowment). Long range effects from *in vitro* to *in vivo*. **M. Gruebele**

9:40 PHYS **79.** Revealing large-amplitude motions using local probes. **C.H. Londergan**

10:00 Intermission.

10:15 PHYS **80.** Protein dynamics by femtosecond x-ray solution scattering and absorption. **M. Cammarata**, L. Balducci, M. Levantino

10:45 PHYS **81.** Biopolymer elasticities via terahertz spectroscopy. **T.M. Korter**

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photoreceptor Activity: Non-Rhodopsin Photosensors

K. Glusac, D. S. Larsen, *Organizers*

M. Olivucci, *Organizer, Presiding*

8:00 PHYS **82.** Ultrafast biological photomachine: Watching DNA repair in real time. **D. Zhong**

8:30 PHYS **83.** Using light as a trigger to understand biological mechanisms. **M. Sans**, D.C. Monteiro, J.J. Doyle, B.A. Yorke, A.R. Pearson

9:00 PHYS **84.** Unfolding of the C-terminal Ja helix in the LOV2 photoreceptor domain observed by time-resolved vibrational spectroscopy. P. Konold, T. Mathes, J. Weissenborn, M. Groot, P. Hegemann, **J. Kennis**

9:30 Intermission.

9:50 PHYS **85.** Ground state and photo-induced electron transfer in cryptochromes. R. Tazhigulov, **K.B. Bravaya**

10:20 PHYS **86.** Structure-guided design of infrared fluorophores based on the sunlight-driven photoreceptor phytochrome. **K.T. Forest**

10:50 PHYS **87.** Correlating secondary protein dynamics with cryokinetics measurements in cyanobacteriochromes. **D.S. Larsen**, N. Rockwell, J. Lagarias, P. Kim

11:10 PHYS **88.** Revealing the molecular identity of cryptochrome photoactivation reaction. **I. Solov'yov**

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Ab Initio & DFT

Cosponsored by COMP

O. V. Prezhdo, *Organizer*

A. V. Akimov, *Organizer, Presiding*

8:00 PHYS **89.** Highly accurate and efficient quantum chemical method based on non-orthogonal localized molecular orbitals. W. Yang, **F. Gu**

8:40 PHYS **90.** Ab Initio multiple spawning molecular dynamics with DFT for intersystem crossings. **D. Fedorov**, S.A. Varganov

9:00 PHYS **91.** Linear scaling calculations with the divide-and-conquer method and with non-orthogonal localized molecular orbitals. **W. Yang**

9:40 Intermission.

9:55 PHYS **92.** Parallel electron dynamics calculations with linear system-size scaling using the time-dependent Hartree-Fock method. **E. Rudberg**

10:35 PHYS **93.** Large-scale real-time TDDFT for studying non-equilibrium electron dynamics in condensed matters: Prospects and challenges in simulating extended systems. **Y. Kanai**, D. Yost, Y. Yao

11:15 PHYS **94.** Multi-petaflop/s quantum molecular dynamics simulations. **A. Nakano**

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Peter Debye Award in Physical Chemistry: Symposium in honor of Bruce J. Berne

Cosponsored by PRES

J. E. Shea, *Organizer*

G. Hummer, *Presiding*

8:00 PHYS **95. Award Address** (Peter Debye Award in Physical Chemistry sponsored by DuPont). Enhanced sampling for thermodynamics and kinetics of ligand-protein binding and unbinding. **B.J. Berne**

8:35 PHYS **96.** Use of molecular dynamics simulations in structure based drug discovery. **R. Friesner**

9:10 PHYS **97.** Free energy simulations of protein-ligand binding and solvation at the interface. **R.M. Levy**

9:45 PHYS **98.** How and when does a drug leave the binding pocket of a host protein. **P. Tiwary**

10:20 Intermission.

10:30 PHYS **99.** Molecular dynamics simulations of protein dynamics from femtoseconds to milliseconds. **G. Hummer**

11:05 PHYS **100.** Ultra-Coarse-Graining and its applications. **G.A. Voth**

11:40 PHYS **101.** Orderphobic effect: A general mechanism for membrane mediated forces between proteins. **D. Chandler**, K. Mandadapu

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Methods

A. T. Krummel, N. E. Levinger, *Organizers*

R. Kumar, *Presiding*

8:20 PHYS **102.** Chemical dynamics in Stochastic Hard Collision (SHC) solvents. **R. Hernandez**

9:00 PHYS **103.** Computing multi-dimensional optical spectra from classical trajectories. **R.F. Loring**

9:20 PHYS **104.** Collective behavior of nonequilibrium, nano-confined fluids. **D. Limmer**

10:00 Intermission.

10:20 PHYS **105.** Tests for, origins of, and corrections to non-Gaussian statistics. A.J. Schile, **W.H. Thompson**

11:00 PHYS **106.** Local structural dynamics revealed by solute-pump/solvent-probe spectroscopy. **X. Sun**, B.M. Ladanyi, R.M. Stratt

11:20 PHYS **107.** Coarse-graining of molecular liquids with integral equation theory. **M. Guenza**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Astrophysics of Ice & Dust

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

R. L. Hudson, *Presiding*

8:00 PHYS **108.** Production mechanisms for complex interstellar molecules. **E. Herbst**, C.N. Shingledecker

8:45 PHYS **109.** Thermally induced low temperature fragmentation reaction in solid phase: Possible answers to the non-detection of some interstellar chemical species. **L. Krim**

9:30 PHYS **110.** Ortho-to-para ratios of hydrogen molecules desorbed from ice at around 10 K: What happens on cosmic ice dust? **N. Watanabe**, H. Ueta, T. Hama, A. Kouchi

10:15 PHYS **111.** Gas-phase chemistry above interstellar and cometary ice analogs. **S.L. Widicus Weaver**, A.J. Mesko, H. Smith, S.N. Milam

10:45 PHYS **112.** Extreme Isotope Ratios in Meteoritic Material: A Gas-Phase Interstellar Origin? **L.M. Ziurys**, D.T. Halfen, T. Zega

Advanced X-Ray Techniques for Catalyst Characterization

Electro- & Photo-Catalysis

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Sponsored by COMP, Cosponsored by PHYS

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

Coherent Multidimensional Spectroscopy in Materials Science

Sponsored by ANYL, Cosponsored by PHYS

MONDAY AFTERNOON

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Cosponsored by INOR

S. Corcelli, *Organizer*

E. Blair, *Presiding*

1:30 PHYS **113.** Probing vibrational coupling and relaxation in cyanide-bridged transition metal mixed-valence complexes. **M.H. Khalil**

2:10 PHYS **114.** Electrostatic and electrodynamic fields in lipid bilayer membranes. **L.J. Webb**

2:50 Intermission.

3:10 PHYS **115.** Voltage-gated switching of anion-molecule assemblies at interfaces and in solution. **A.H. Flood**

3:50 PHYS **116.** Radical chemistry and charge manipulation with an atomic force microscope. **L. Gross**, B. Schuler, N. Pavliček, S. Fatayer, Z. Majzik, N. Moll, G. Meyer

4:30 PHYS **117.** Revisiting the structure-properties relation in charge transport across large area molecular tunneling junctions. **J. Chen**, H. Yoon, M. Thuo

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Dynamics Relevant to Electron & Proton Transfer

A. V. Benderskii, J. Dawlaty, *Organizers*

S. T. Roberts, *Presiding*

1:30 PHYS **118.** Proton coupled electron transfer in photosynthetic oxygen evolution: Role for internal water and hydrogen bonded networks. **B.A. Barry**, U. Brahmachari, Z. Guo

2:10 PHYS **119.** Hydrated excess proton-ultrafast vibrational dynamics of the Zundel cation $H_5O_2^+$. F. Dahms, R. Costard, B. Fingerhut, E. Pines, **E. Nibbering**, T. Elsaesser

2:30 PHYS **120.** Dissecting the molecular structure and dynamics of aqueous systems through many-body molecular dynamics simulations. **F. Paesani**

3:10 Intermission.

3:30 PHYS **121.** Panoramic portrait of photochemical events in solution and proteins captured by femtosecond Raman spectroscopy. L. Tang, B.G. Oscar, Y. Wang, L. Zhu, W. Liu, **C. Fang**

4:10 PHYS **122.** Time-resolved infrared spectroscopy as a probe of nonequilibrium hydrogen-bond dynamics: A mixed quantum-classical study of alcohols in liquid solution. **E. Geva**

4:30 PHYS **123.** Alteration of photoacidic behavior of pyrenol dyes covalently bound in the nanoconfined, electrostatically-complicated tips of asymmetric nanopores. **C. Sanborn**, J.V. Chacko, S. Ardo

4:50 PHYS **124.** Photoinduced charge separation and recombination in DNA strands. **B. Kohler**

Section C

Parc 55 San Francisco

Hearst

Long Range Correlated Motions in Proteins

Dynamical Measurements & Calculations using Protein Crystals

A. Markelz, *Organizer*

M. Cammarata, *Presiding*

1:30 PHYS **125.** Fast and ultrafast structural investigations of trans to cis isomerizations in photoreactive proteins. **M. Schmidt**

2:00 PHYS **126.** Ultra-fast time-resolved serial femtosecond crystallography on myoglobin ligand dissociation. **I. Schlichting**

2:30 PHYS **127.** Photo-intermediate State Dependence of Picosecond Motions in Photoactive Proteins. **Y. Deng**, M. Xu, H. Liu, K. Niessen, M. Schmidt, R.E. Blankenship, A. Markelz

2:50 Intermission.

3:05 PHYS **128.** Non-thermal effect of terahertz radiation on crystals of lysozyme at room temperature and bovine trypsin at 100 K. **G. Katona**, I. Lundholm, W.Y. Wahlgren, M. Garcia Bonete, H. Rodilla, J. Stake, J. Vukusic, A. Duelli, H. Bassereh, G. Bourenkov, T. Schneider, R. Friedman

3:35 PHYS **129.** Effect of intermolecular interactions on mixing of intermolecular and intramolecular vibrations: Terahertz spectroscopy and solid-state density functional theory. F. Zhang, H. Wang, K. Tominaga, **M. Hayashi**

4:05 PHYS **130.** Mutation induced structure changes in histone proteins. **T. Yu**, G.C. Schatz, J. Licht

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Fragmentation & Linear Scaling: Semiempirical & DFTB

Cosponsored by COMP

A. V. Akimov, *Organizer*

O. V. Prezhdo, *Organizer, Presiding*

1:30 PHYS **131.** Nonadiabatic molecular dynamics with tight-binding fragment molecular orbitals. **A.V. Akimov**

2:10 PHYS **132.** Fragment orbital-based surface hopping for simulation of charge carrier transport in materials and biomolecules. A. Carof, L. Scalfi, **J. Blumberger**

2:50 PHYS **133.** Nonadiabatic molecular mechanics/extended Hückel excited state quantum dynamics method. **L.G. Rego**, R. Oliboni, A. Torres, G. Bortolini

3:30 Intermission.

3:45 PHYS **134.** Chemical reaction simulations treated by linear-scaling Divide-and-Conquer Type Density-Functional Based Tight-Binding Molecular Dynamics (DC-DFTB-MD) method. **H. Nakai**

4:25 PHYS **135.** QM/MM simulations of electron/exciton transfer reactions. **M. Elstner**

5:05 PHYS **136.** Force field accelerated density functional theory molecular dynamics for simulation of reactive systems at extreme conditions. **R. Lindsey**, N. Goldman, L.E. Fried

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids: Symposium in honor of Salvatore Torquato

Cosponsored by PRES

J. E. Shea, *Organizer*

P. G. Debenedetti, *Presiding*

1:30 Introductory Remarks.

1:35 PHYS **137.** Hard spheres under gravity. **F. Stillinger**

2:15 PHYS **138.** Inverse design of interactions for assembly. **T. Truskett**

2:55 PHYS **139.** Structure and dynamics in cold aqueous clusters: Quantum and classical perspectives. **P.J. Rossky**

3:35 Intermission.

3:50 PHYS **140.** Nano-scale drying and hydration phenomena. **P.G. Debenedetti**

4:30 PHYS **141. Award Address** (Joel Henry Hildebrand Award in the Theoretical & Experimental Chemistry of Liquids sponsored by ExxonMobil Research & Engineering Company). Disordered hyperuniform materials: New states of amorphous matter. **S. Torquato**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Ionic Liquids

A. T. Krummel, N. E. Levinger, *Organizers*

M. Guenza, *Presiding*

1:30 PHYS **142.** Molecular geometries and electronic structures of ionic liquids: Bulk, vacuum interfaces, and ultrathin films. **E. Castner**

2:10 PHYS **143.** Heterogeneity in solvation by an ionic liquid: A qualitative distinction between inertial and diffusive dynamics. S. Verma, S. Corcelli, **M.A. Berg**

2:30 PHYS **144.** Solute dynamics in ionic liquids: Experiment and simulation. **M. Maroncelli**, C. Rumble, B. Conway, C. Uitvlugt

3:10 Intermission.

3:30 PHYS **145.** Dynamics and vibrational spectroscopy of solutes in ionic liquids. **S. Corcelli**

4:10 PHYS **146.** Photo-induced electron transfer by ions in ionic liquids. **B. Wu**, M. Maroncelli, E. Castner

4:30 PHYS **147.** Carbon dioxide dynamics in room temperature ionic liquids and supported ionic liquid membranes: 2D IR and polarization selective pump-prove experiments. **M.D. Fayer**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Kuiper Belt Objects & Comets

M. S. Gudipati, *Organizer*

R. Kaiser, *Organizer, Presiding*

N. Watanabe, *Presiding*

1:30 PHYS **148.** Chemistry in protoplanetary disks. **T.K. Henning**

2:15 PHYS **149.** Chemical evolution of organic materials from protoplanetary disk to small bodies recorded in Antarctic micrometeorites. **H. Yabuta**

3:00 PHYS **150.** Energetic gas-surface encounters at ice interfaces. G. Langlois, R.S. Thompson, W. Li, K. Gibson, D.R. Killelea, H. Yuan, **S.J. Sibener**

3:45 PHYS **151.** Adsorption, diffusion, aggregation, and desorption of simple molecules (CO_2, CO, O_2, etc.) on interstellar ice analogs. **G. Vidali**, J. He, S. Emtiaz

4:30 PHYS **152.** Synthesizing the basic PAH unit. **B. Sivaraman**

Advanced X-Ray Techniques for Catalyst Characterization

New Methodologies

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

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LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

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Catalytic Materials from Molecular Insight

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Strong Electron Correlation & Nonadiabatic Dynamics

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Coherent Multidimensional Spectroscopy in Materials Science

Sponsored by ANYL, Cosponsored by PHYS

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

J. E. Shea, *Organizer*

8:00 - 10:00

39, 59. See previous listings.

169, 220, 241, 247, 338, 367-368, 380-381, 396, 453, 465, 470, 478, 493, 499, 505, 511, 515, 523, 532, 541. See subsequent listings.

TUESDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Applications & Devices

Cosponsored by INOR

S. Corcelli, *Organizer*

S. Roy, *Presiding*

8:00 PHYS **153.** Investigation of quantum-dot cellular automata networks using a quantum annealing processor. J. Retallick, **K. Walus**

8:40 PHYS **154.** Multistable mixed-valence molecular entities for quantum cellular automata: Vibronic localization in isolated and coupled cells. **B. Tsukerblat**, A. Palii

9:20 Intermission.

9:40 PHYS **155.** Fully-quantum, non-equilibrium model of vibration-coupled, electric-field-driven electron transfer in mixed-valence molecules. **E. Blair**

‡ *Cooperative Cosponsorship*

10:20 PHYS **156.** Properties of multiple silicon atom artificial molecules on a silicon surface. **R.A. Wolkow**

11:00 PHYS **157.** Mixed-valence molecules could be the replacement for the transistor. **C. Lent**

Section B

Parc 55 San Francisco

Mission I

Spectroscopy of Complex Systems

Exciton Dynamics & Dissociation in Heterogeneous Systems

A. V. Benderskii, J. Dawlaty, *Organizers*

P. B. Petersen, *Presiding*

8:00 PHYS **158.** Extracting triplet excitons produced by singlet exciton fission from perylenediimide thin films. A.K. Le, J.A. Bender, A.P. Moon, R. Pandey, **S.T. Roberts**

8:40 PHYS **159.** Resonance Raman study of exciton-phonon coupling in CdSe and ZnSe quantum dots and their alloys. K. Gong, D.F. Kelley, **A.M. Kelley**

9:00 PHYS **160.** Probes of structure, disorder, and dynamics of excited states in conjugated materials. **A.E. Bragg**

9:40 Intermission.

10:00 PHYS **161.** Probing the mechanism of singlet fission with femtosecond stimulated Raman spectroscopy. **R.R. Frontiera**, S.M. Hart, W.R. Silva, K. Bera, S. Kwang, A. Cassabaum

10:40 PHYS **162.** Interfacial disorder drives charge separation in molecular semiconductors. **A. Willard**, C. Lee, L. Shi

11:20 PHYS **163.** Intermolecular vibronic coherence transfer in an organic electrode material. **A. Rury**, J. Dawlaty

11:40 PHYS **164.** When a single structure is not sufficient: Effect of thermal deformation on excitonic properties of semiconductor nanoparticles. J. Scher, A. Srihari, M.G. Bayne, S. Nangia, **A. Chakraborty**

Section C

Parc 55 San Francisco

Hearst

Long Range Correlated Motions in Proteins

Catalysis

A. Markelz, *Organizer*

A. Grossfield, *Presiding*

9:00 PHYS **165.** Motions in proteins and drug design. **J. Smith**

9:30 PHYS **166.** Evolution and designing enzymes for rapid protein dynamics and catalysis. **S.D. Schwartz**

10:00 PHYS **167.** Sensitivity to protein vibration directionality and the relation to function. **K.A. Niessen**, M. Xu, Y. Deng, E. Snell, A. Markelz

10:20 PHYS **168.** Role of statistical fluctuations and electrostatics in the improvements of de novo enzyme catalysis. **T.L. Head-Gordon**

10:50 PHYS **169.** Withdrawn.

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Simulations in Materials Systems

Cosponsored by COMP

A. V. Akimov, *Organizer*

O. V. Prezhdo, *Organizer, Presiding*

8:00 PHYS **170.** Relating chromophoric and structural disorder in conjugated polymers. **L. Simine**, P.J. Rossky

8:20 PHYS **171.** Dynamics of organic materials with optical activity: Advances, appraisal, applications. **M. Barbatti**

9:00 PHYS **172.** Charge transfer and singlet fission quantum dynamics in organic photovoltaic. **P. Huo**

9:40 PHYS **173.** Theoretical investigation of electron-nuclear dynamics in the neutral and cationic $[Au_{25}(SH)_{18}]^{q}$ [q = 0, +1] thiolate-protected gold nanoclusters. **R.D. Senanayake**, A.V. Akimov, C.M. Aikens

10:00 Intermission.

10:15 PHYS **174.** Mapping nuclear dynamics in nonadiabatic molecular dynamics simulations. **G. Tao**

10:55 PHYS **175.** Theoretical investigation of novel CdSe/$Cd_{1-x}Zn_xS$ seeded nanorods exhibiting high quantum-yield, high polarization, and minimal blinking. I. Hadar, **J.P. Philbin**, Y. Panfil, H. Eshet, E. Rabani, U. Banin

11:15 PHYS **176.** Strong binding of CdSe quantum dots to single-walled carbon nanotubes. **B. Rudshteyn**, S. Azoz, W. Ding, F. Ren, M. Askerka, A. Matula, N. Marinkovic, G.L. Haller, L. Pfefferle, V.S. Batista

11:35 PHYS **177.** Exciton transport in disordered molecular systems in couple with the quantum fluctuating electromagnetic field of metal surface. **X. Chen**, A. Poudel, M.A. Ratner

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

ACS Award in Theoretical Chemistry: Symposium in honor of Peter Pulay

Cosponsored by PRES

J. E. Shea, *Organizer*

S. Hirata, *Presiding*

8:00 PHYS **178.** Paradigm changes in the methodology of computational quantum chemistry: A tribute to the contributions by Peter Pulay. **W.E. Meyer**

8:30 PHYS **179.** Density cumulant functional theory. **H.F. Schaefer**

9:00 PHYS **180.** 34 years of local electron correlation: From Peter Pulay's pioneering work to the state-of-the-art. **H. Werner**

9:30 Intermission.

10:00 PHYS **181.** Merging symmetry projection methods with coupled cluster theory. **G.E. Scuseria**

10:30 PHYS **182.** Scalable electron-correlation methods and instabilities versus strong correlation: A legacy of Peter Pulay. **S. Hirata**

11:00 PHYS **183. Award Address** (ACS Award in Theoretical Chemistry sponsored by the ACS Division of Physical Chemistry). Molecular properties from quantum mechanical calculations 1967 - 2017: Synergy, successes, and challenges. **P. Pulay**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Extreme Environments

A. T. Krummel, N. E. Levinger, *Organizers*

M. McCullagh, *Presiding*

8:00 PHYS **184.** Why do isotropic liquid crystals resemble supercooled liquids? **R.M. Stratt**

8:40 PHYS **185.** Relaxation and self-diffusion of liquids and supercooled liquids derived from picosecond timescale dynamics. **M.T. Cicerone**, M. Tyagi, M. Zhi, J.S. Bender

9:00 PHYS **186.** Fundamental differences between glassy dynamics in two and three dimensions. **G. Szamel**

9:20 PHYS **187.** Wetting behavior of alkane–water nanodroplets and planar interfaces. P. Neupane, F. Hrahsheh, **G. Wilemski**

10:00 Intermission.

10:20 PHYS **188.** Supercooled water: Three-body interactions, IR spectra in no man's land, and the liquid-liquid critical point. **J.L. Skinner**

11:00 PHYS **189.** Electronically coarse grained model, including all quantum mechanical fluctuations necessary for long-range forces, describes water's properties from ice to the supercritical regime. **G.J. Martyna**

11:20 PHYS **190.** Thermodynamic forces between plant cell wall constituents. **M.S. Skaf**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Condensed Materials in the Outer Solar System

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

B. L. Henderson, *Presiding*

8:00 PHYS **191.** Chemistry and processes in the Pluto system. **W. Grundy**, D. Cruikshank, C. Olkin, S. Stern, K. Ennico-Smith, L. Young, H.A. Weaver

8:45 PHYS **192.** Links between the ices of comet 67P/Churyumov-Gerasimenko and the interstellar medium from Rosetta/ROSINA observations. **M. Rubin**, K. Altwegg, H. Balsiger, J. Berthelier, M. Combi, J. De Keyser, B. Fiethe, S. Fuselier, S. Gasc, T. Gombosi, K. Hansen, U. Mall, H. Rème, M. Schuhmann, I. Schroeder, T. Sémon, C. Tzou, J.H. Waite, S. Wampfler, P. Wurz

9:30 PHYS **193.** Aerosol impact spectrometer – A variable velocity nanoparticle accelerator. **R.E. Continetti**

10:15 PHYS **194.** Self-Assembly of prebiotic organic materials from impact events of amino acid solutions. **N. Goldman**

10:45 PHYS **195.** Comparison of gas phase and condensed phase species: Sgr B2(N) vs. Comet 67P. **D.T. Halfen**, J. Bernal, L.M. Ziurys

11:15 PHYS **196.** Results from recent experiments on electron-stimulated desorption from icy & rocky surfaces. **C. Bennett**, M.J. Poston, T.M. Orlando

Advanced X-Ray Techniques for Catalyst Characterization

New Methodologies

Sponsored by CATL, Cosponsored by PHYS

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Theory & Experiment

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Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG² and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

TUESDAY AFTERNOON

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Theory & Modeling

Cosponsored by INOR

S. Corcelli, *Organizer*

C. Lent, *Presiding*

1:30 PHYS **197.** Information propagation in molecular field coupled nanocomputing logic. **M. Graziano**, R. Wang, G. Piccinini

2:10 PHYS **198.** Organic semiconductors: Singlets and triplets and charges, oh my! **T.A. Van Voorhis**, P. de Silva, T. Zhu

2:50 Intermission.

3:10 PHYS **199.** Theoretical study of dyamics in molecular junctions: Effects of molecule and electrode microstructure on electron transport. A. Becker, J. Kern, **S. Roy**

3:50 PHYS **200.** Practical approaches for studying photochemistry of large molecules in solution and some nice applications. **J.E. Subotnik**, A. Jain, G.R. Medders

4:30 PHYS **201.** Nonadiabatic electron-transfer in mixed-valence molecules. **S. Corcelli**

Section B

Parc 55 San Francisco

Mission I

Spectroscopy of Complex Systems

Exciton Dynamics & Dissociation in Heterogeneous Systems

A. V. Benderskii, J. Dawlaty, *Organizers*

A. Rury, *Presiding*

1:30 PHYS **202.** Multiresonant coherent multidimensional spectroscopy of cobalamin. **J.C. Wright**, J. Handali, N. Neff-Mallon

2:10 PHYS **203.** Two dimensional spectroscopy of photosynthetic light harvesting antennae. **G.S. Engel**

2:30 PHYS **204.** Mixed quantum/semiclassical simulations of ultrafast dynamics and spectroscopic signals. **J.A. Cina**, P.A. Kovac

3:10 Intermission.

3:30 PHYS **205.** Harnessing shared vibrations to control energy transfer. **D.M. Jonas**

4:10 PHYS **206.** Accessing excitonic structure of a photosynthetic Fenna-Matthews-Olson pigment-protein complex by time-resolved circular dichroism spectroscopy. **S. Savikhin**, V. Stadnytskyi, G. Orf, R.E. Blankenship

4:30 PHYS **207.** Withdrawn.

4:50 PHYS **208.** Ultrafast 2D white light spatial imaging of single nano-structures. **A.C. Jones**, N.M. Kearns, M.T. Zanni

5:10 PHYS **209.** Probing ultrafast electron dynamics at surfaces using soft x-ray transient reflectivity spectroscopy. **L. Baker**, J. Husek, S. Biswas, A. Cirri

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Photoreceptor Activity: Rhodopsins Photosensors

K. Glusac, D. S. Larsen, *Organizers*

M. Olivucci, *Organizer, Presiding*

1:30 PHYS **210.** Photoactivation mechanisms of rhodopsins from time-resolved optical absorption spectroscopy. **D.S. Kliger**

2:10 PHYS **211.** Unexpected rhodopsin functions initiated by common retinal photoisomerization. **H. Kandori**

2:50 PHYS **212.** Evidence for a vibrational phase isotope effect on the photochemistry of vision. **R.A. Mathies**, C. Schnedermann, M. Liebel, K.M. Spillane, P. Kukura, I. Fernandez, J. Lugtenburg

3:30 Intermission.

3:50 PHYS **213.** Effect of point mutations on the ultrafast photo-isomerization of anabaena sensory rhodopsin. **S. Haacke**, D. Agathengelou, J. Leonard, H. Kandori, K. Jung

4:30 PHYS **214.** Understanding and designing color variants of retinal binding proteins by molecular simulations. **S. Hayashi**

Section D

Parc 55 San Francisco

Divisadero

Quantum Dynamics in Large Scale Systems

Simulations in Biological Systems

Cosponsored by COMP

A. V. Akimov, *Organizer*

O. V. Prezhdo, *Organizer, Presiding*

1:30 PHYS **215.** Importance of polarizable embedding in biological systems: Excitonic interactions in photosynthetic proteins. **L.V. Slipchenko**

2:10 PHYS **216.** Improving density functional tight binding predictions of free energy surfaces for peptide condensation reactions in solution. **M. Kroonblawd**, N. Goldman

2:30 PHYS **217.** Energy profiles for modeling transient kinetic studies of chemical reactions in proteins. **A. Nemukhin**

3:10 Intermission.

3:25 PHYS **218.** QM/MM dynamics for metalloproteins, so far without quantum dynamics. C.E. Valdez, M.R. Nechay, A. Morgenstern, M. Eberhart, **A. Alexandrova**

4:05 PHYS **219.** Quantum mechanical force fields for condensed phase molecular simulations. **D.M. York**

4:45 PHYS **220.** Single ion solvation free energies with ab initio molecular dynamics. **T.T. Duignan**, M.D. Baer, G.K. Schenter, C.J. Mundy

5:05 PHYS **221.** Thermoelectric effect and its dependence on molecular length and sequence in single DNA molecules. **Y. Li**, L. Xiang, J.L. Palma, Y. Asai, N. Tao

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

E. Bright Wilson Award: Symposium in honor of David J. Nesbitt

Cosponsored by PRES

J. E. Shea, *Organizer*

M. I. Lester, *Presiding*

1:30 PHYS **222.** Always acetylene! **R. Field**, J. Baraban, B. Changala, Z. Du, J. Jiang, A. Merer, A. Muthike, C. Saladrigas

2:05 PHYS **223.** Unimolecular decay of Criegee intermediates to hydroxyl radical products. **M.I. Lester**

2:40 PHYS **224. Award Address** (E. Bright Wilson Award in Spectroscopy sponsored by the ACS Division of Physical Chemistry). Good, good, good rovibrations! **D.J. Nesbitt**

3:25 Intermission.

3:45 PHYS **225.** Properties of molecular clusters from broadband molecular rotational spectroscopy. **B.H. Pate**

4:20 PHYS **226.** Formation of exotic networks of water clusters in helium droplets facilitated by the presence of neon atoms. **G.E. Douberly**, S. Xantheas

4:55 PHYS **227.** Spectroscopic resolution attosecond measurements. **S.R. Leone**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Interfaces

A. T. Krummel, N. E. Levinger, *Organizers*

M. Berg, *Presiding*

1:30 PHYS **228.** Chemical processes at environmental water-air interfaces. **V. Vaida**, E. Griffith, R. Rapf, R. Perkins

2:10 PHYS **229.** Quantifying the catalyst's role in inverse phase transfer catalysis with computer simulations. **J.J. Karnes**, I. Benjamin

2:30 PHYS **230.** Visualization of charge motion in nanostructures with pump-probe microscopy. **J.M. Papanikolas**

3:10 Intermission.

3:30 PHYS **231.** Ice: The common solid we hardly know. **M.J. Shultz**, P.J. Bisson, J. Marmolejos, A. Brumberg

4:10 PHYS **232.** Solvation dynamics of aqueous solutions in extreme hydrophilic confinement. **R.C. Remsing**

4:30 PHYS **233.** Dynamics and structure of water in confined environments. **A. Luzar**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Chemistry of Condensates on the Terrestrial Planets

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

N. Goldman, *Presiding*

1:30 PHYS **234.** Quantum chemistry and ab initio molecular dynamics simulations of reactive chemistry in ionized clusters: From acetylene clusters to aromatics. T. Stein, M. Ahmed, **M.P. Head-Gordon**

2:15 PHYS **235.** Nucleobase synthesis via UV-induced oxidation of their precursors in astrophysical ices: A quantum chemical perspective. **P. Bera**, T. Stein, M.P. Head-Gordon, T.J. Lee

3:00 PHYS **236.** Theoretical cluster studies of charge shift reactions in astrophysical ices. **D.E. Woon**

3:45 PHYS **237.** Formation of formamide NH_2CHO catalyzed by icy grain particles: Atomistic insights from quantum chemical simulations. **A. Rimola**, V. Taquet, C. Ceccarelli, N. Balucani, P. Ugliengo

4:15 PHYS **238.** Adsorption and catalysis of noble gas atoms and electrons on PAH surfaces. **R.C. Fortenberry**, G.T. Filipek, II, C.M. Novak, M.M. Moore, M.L. Theis, T.J. Lee

Catalytic Materials from Molecular Insight

Sponsored by COMP, Cosponsored by CATL, MPPG‡ and PHYS

Strong Electron Correlation & Nonadiabatic Dynamics

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY MORNING

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Synthesis

Cosponsored by INOR

S. Corcelli, *Organizer*

M. Lieberman, *Presiding*

8:00 PHYS **239.** Structural insight into electronic communication and energy transfer in metal organic framework arrays. **A.J. Morris**, J.M. Rowe

8:40 PHYS **240.** Nano-Confinement inside molecular metal oxide clusters: Dynamics and modified encapsulation behavior. **P. Yin**

9:00 PHYS **241.** Investigating the transformations of polyoxoanions using mass spectrometry and molecular dynamics. **L. Vilà Nadal**, L. Cronin

9:20 PHYS **242.** Charge localization vs delocalization in tetranuclear mixed-valence complexes: A spectroscopic study. **C. Lapinte**, J. Hamon, R. Makhoul, P. Hamon

10:00 Intermission.

10:20 PHYS **243.** Closo-$Si_{12}C_{12}$ Molecule from cluster to crystal: Structure and properties of closo-$Si_{12}C_{12}$ siloxane polymers. **X.F. Duan**, L.W. Burggraf

10:40 PHYS **244.** Layer-by-layer assembled MOFs. Building ordered chromophoric arrays and propagating molecular excitons. S. Goswami, O.K. Farha, **J.T. Hupp**

11:20 PHYS **245.** Lanthanide-based single-molecule magnets with high blocking temperatures. S. Demir, C. Gould, L.E. Darago, M.I. Gonzalez, K.R. Meihaus, J. Zadrozny, M. Nippe, J.D. Rinehart, **J.R. Long**

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Effects of Nanoconfinement & Local Asymmetry on Dynamics & Chemistry: Local E-Fields

A. V. Benderskii, J. Dawlaty, *Organizers*

A. Rury, *Presiding*

8:00 PHYS **246.** Electric fields and enzyme catalysis. **S.G. Boxer**

8:40 PHYS **247.** Vibrational sum frequency generation Stark shift spectroscopy: Measuring the electric field at a metal-dielectric interface. **S.A. Sorenson**, J. Patrow, J. Dawlaty

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

‡ *Cooperative Cosponsorship*

9:00 PHYS **248.** Probing electrostatics along the catalytic cycle of an enzyme with site-specific nitrile probes. **S. Hammes-Schiffer**

9:40 Intermission.

10:00 PHYS **249.** Calibrating the vibrational Stark effect of nitrile probes in the presence of hydrogen bonding with independently measured electric fields in green fluorescent protein. **L.J. Webb**

10:40 PHYS **250.** Non-linear SFG spectroscopy of mineral/water interfaces containing electrolytes & tera-hertz spectroscopy in liquid water: A DFT-MD theoretical perspective. **M.P. Gaigeot**

11:00 PHYS **251.** Atomistic electrodynamic-quantum mechanical approaches for simulating surface-enhanced hyper-Raman scattering: Theory and application. **Z. Hu**, D. Chulhai, L. Jensen

11:20 PHYS **252.** Attosecond quantum kinetics of photoexcited Germanium. **P. Kraus**, C. Kaplan, M.W. Zuerch, H. Chang, L.J. Borja, M.F. Jager, S. Cushing, D.M. Neumark, S.R. Leone

11:40 PHYS **253.** Driving delocalized dynamics using the orbital angular momentum of light. **B.S. Rolczynski**, P. Navotnaya, G.S. Engel

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Excited-State Dynamics & Microscopy

K. Glusac, D. S. Larsen, M. Olivucci, *Organizers*

S. Haacke, *Presiding*

8:00 PHYS **254.** Electronic energy redistribution in conjugated molecules and the effect of an energy gradient. **V.D. Kleiman**

8:30 PHYS **255.** Space- and time-resolved spectroscopy of energy transfer. **T. Brixner**

9:00 PHYS **256.** Ultrafast vibronic microspectroscopy of nanostructured electronic materials. C. Schnedermann, J. Lim, A. Rao, **P. Kukura**

9:30 PHYS **257.** Ultrafast spectroscopic observation of cysteine-based redox regulation of coherent energy transfer in a photosynthetic antenna complex. **J.P. Otto**, M.A. Allodi, R.G. Saer, S.H. Sohail, R.E. Blankenship, G.S. Engel

9:50 PHYS **258.** Resolving the detailed 2D spectral structure of the Fenna-Matthews-Olson complex. **B.S. Rolczynski**, S. Yeh, P. Navotnaya, K. Ashraf, A.T. Gardiner, R.J. Cogdell, G.S. Engel

10:10 Intermission.

10:30 PHYS **259.** Electronic and geometric dynamics of transition metal complexes for solar energy conversion. **L.X. Chen**, M. Shelby, D. Hayes, R. Hadt, P. Kim, S. Brown-Xu, J. Hong, M. Kelley

11:00 PHYS **260.** Torsional dynamics, intramolecular charge transfer, and solvent friction in the S_2 ($1^1B_u^+$) excited state of peridinin: A mechanism for enhanced mid-visible light harvesting in the peridinin–chlorophyll a protein. **W.F. Beck**, J.D. Roscioli, S. Ghosh, M.M. Bishop, A.M. LaFountain, H.A. Frank

11:20 PHYS **261.** Probing the dynamics of higher-lying excited states. **C.G. Elles**, T.J. Quincy, M.S. Barclay

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Metamaterials & Information Technology

P. K. Jain, *Organizer*

C. J. Murphy, *Organizer, Presiding*

8:00 PHYS **262.** Film-Coupled nanocubes: From ultrafast spontaneous emission to perfect absorbers. **M.H. Mikkelsen**

8:35 PHYS **263.** Dynamic plasmonic metamaterials with broken symmetry created via directed self-assembly. **D.B. Litt**, M.R. Jones, M. Hentschel, P. Alivisatos

8:55 PHYS **264.** Towards all-optical chiral resolution with achiral plasmonic and dielectric nanostructures. **J. Dionne**

9:30 PHYS **265.** Magneto-Optical response of cobalt interacting with plasmonic nanoparticle superlattices. **M.B. Ross**, C.A. Mirkin, G.C. Schatz

9:50 Intermission.

10:05 PHYS **266.** Heat-assisted magnetic recording: Next-generation mass storage technology. **M. Re**, J. Thiele, G. Ju, C. Rea, T. Rausch, M. Siegler, E. Gage

10:40 PHYS **267.** Near field thermal imaging: Sub-diffraction and steady state thermal measurements on optically excited gold nanostructures. S. Baral, A. Rafiei Miandashti, **H.H. Richardson**

11:00 PHYS **268.** Plasmonic transition metal nitrides for harsh-environment photonic applications. U. Guler, H. Reddy, K. Chaudhury, A. Naldoni, A. Kildishev, V. Shalaev, **A. Boltasseva**

11:35 PHYS **269.** Far-field supperresolution detection of plasmonic near-fields. **R.C. Boutelle**, D. Neuhauser, S. Weiss

Section E

Parc 55 San Francisco

Embarcadero

PHYS Division Awards Symposium

Francis P. Garvan–John M. Olin Medal: Symposium in honor of Barbara J. Finlayson-Pitt

Cosponsored by PRES

J. E. Shea, *Organizer*

S. A. Nizkorodov, *Presiding*

8:00 Introductory Remarks.

8:05 PHYS **270. Award Address** (Francis P. Garvan–John M. Olin Medal sponsored by Francis P. Garvan–John M. Olin Medal Endowment). From active molecules to atmospheric models: The central role of molecular level understanding in improving human health and welfare. **B.J. Finlayson Pitts**

8:40 PHYS **271.** Towards molecular-level understanding of growth, formation and properties of atmospheric acid-base particles. **R.B. Gerber**, J. Xu, K. Arquero, B.J. Finlayson Pitts

9:05 PHYS **272.** Atmospheric photochemistry of pyruvic acid and related oxoacids. **V. Vaida**, A. Reed Harris, R. Rapf, R. Perkins

9:30 PHYS **273.** Enhanced reactivity in aqueous aerosols: Why bulk-phase aqueous measurements can mislead us. **D.O. Dehaan**

9:55 Intermission.

10:15 PHYS **274.** Studies of halogen chemistry in the Arctic. **P.B. Shepson**

10:45 PHYS **275.** Molecular dynamics simulation studies of ions and acids at atmospherically relevant aqueous solution-air interfaces. **D. Tobias**

11:10 PHYS **276.** Composition and chemistry of the liquid/vapor interface of aqueous solutions. **J.C. Hemminger**

11:35 PHYS **277.** Organic photochemistry in atmospheric particulate matter. **S.A. Nizkorodov**

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Complex Systems

A. T. Krummel, N. E. Levinger, *Organizers*

R. Remsing, *Presiding*

8:20 PHYS **278.** Biomolecular hydration shells: Dynamics and effect on biochemical function. **D. Laage**

9:00 PHYS **279.** Probing PDI nanoaggregate structures by combining MD simulations & 2D IR spectroscopy. **A.T. Krummel**

9:20 PHYS **280.** Biological water or rather water in biology? **P. Jungwirth**

10:00 Intermission.

10:20 PHYS **281.** Bottom-up treatment of nonpolar solvation for molecular dynamics simulations. P.T. Lake, **M. McCullagh**

11:00 PHYS **282.** Magnesium fluctuations modulate RNA dynamics in riboswitch. **U. Mohanty**

11:20 PHYS **283.** Depolarized light scattering and terahertz absorption of protein solutions. **D.V. Matyushov**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Physical Properties of Condensed Super Volatiles on Pluto: From the New Horizon Mission

M. S. Gudipati, *Organizer*

R. Kaiser, *Organizer, Presiding*

G. Vidali, *Presiding*

8:00 PHYS **284.** Probing molecular growth and charge transfer processes with vacuum ultraviolet mass spectrometry. **M. Ahmed**

8:45 PHYS **285.** Chemical processing in interstellar grains via electron and UV radiation. **B.L. Henderson**, M.S. Gudipati

9:30 PHYS **286.** Photon-stimulated processes on planetary surfaces and in astrophysical environments. **T.M. Orlando**, C. Bennett, J. McLain, M. Sarantos

10:15 PHYS **287.** Chemical functionalization and catalytic activity of polycyclic aromatic hydrocarbons on dust grain surfaces. **L. Hornekaer**, J.H. Jørgensen, A.W. Skov

11:00 PHYS **288.** PAHs, Dust and ice in the solar system. **A. Mattioda**, G. Cruz-Diaz, A. Ricca Bauschlicher, A. de Barros, S. Erickson, P. van Vliet, E. da Silveira, A. Cook

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Dynamics & Modeling of Allosteric Systems

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY AFTERNOON

Section A

Parc 55 San Francisco

Sutro

Multicenter Molecules & Coupled Molecular Assemblies: Synthesis, Characterization & Theory

Experimental Characterization

Cosponsored by INOR

S. Corcelli, *Organizer, Presiding*

1:30 PHYS **289.** Pyrolysis of DNA origami drives carbon atoms into the substrate forming silicon carbide replicas. M.A. Pillers, **M. Lieberman**

2:10 PHYS **290.** Self-assembled crystals that perform molecular rotor-based computations. **E.H. Sykes**, N. Wasio

2:50 Intermission.

3:10 PHYS **291.** Simulation of static and dynamic behavior of molecular quantum-dot cellular automata made of Fe and Ru mixed-valence complexes. **K. Tokunaga**

3:50 PHYS **292.** New reactions in surface chemistry. **F. Rosei**

4:30 PHYS **293.** Electron transfer in the molecular quantum-dot cellular automata: The competition between Coulomb effect and nuclear relaxation. **Y. Lu**, C. Lent

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Effects of Nanoconfinement & Local Asymmetry on Dynamics & Chemistry

A. V. Benderskii, *Organizer*

J. Dawlaty, *Organizer, Presiding*

1:30 PHYS **294.** Dynamics of room temperature ionic liquids measured with two dimensional infrared spectroscopy: The influence of electric fields on observables. **M.D. Fayer**

2:10 PHYS **295.** Environmental effects on the structure of nanoemulsion interfaces. **A. Carpenter**, J. Hensel, R. Ciszewski, B. Schabes, G.L. Richmond

2:30 PHYS **296.** Simulations of the vibrational spectroscopy of water at silica interfaces. J.A. Harvey, P.C. Burris, P. Wimalasiri, **W.H. Thompson**

3:10 Intermission.

3:30 PHYS **297.** Spectroscopic insight into efficiency limiting factors in light-driven H_2 generation using 1D and 2D multicomponent semiconductor/catalyst nanoheterostructures. **T. Lian**

4:10 PHYS **298.** Transition from molecular vibrations to phonons in atomically-precise cadmium selenide quantum dots. A. Beecher, R.A. Dziatko, M.L. Steigerwald, J.S. Owen, **A. Crowther**

4:30 PHYS **299.** Single-molecule exploration of the regulation of photosynthetic light harvesting. **G. Schlau-Cohen**

4:50 PHYS **300.** Linear and nonlinear spectroscopy of multicolor photoresists. Z. Tomova, N. Liaros, S. Gutierrez Razo, H. Ogden, S. Wolf, M. Thum, **J.T. Fourkas**, A.S. Mullin, D. Falvey, J. Petersen

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Exciton Photodynamics: Soft Materials

D. S. Larsen, M. Olivucci, *Organizers*

K. Glusac, *Organizer, Presiding*

1:30 PHYS **301.** What happens to triplet excitons after singlet fission? **C.J. Bardeen**

2:00 PHYS **302.** Introducing a general spin-correct spin-flip configuration interaction method that includes dynamic correlation. **J. Mato**, M.S. Gordon

2:20 PHYS **303.** Excitonic triplet-triplet couplings in dimeric and aggregated dyes: Experiment and theory. **L.V. Slipchenko**, D.A. Hartzler, S. Savikhin

2:40 PHYS **304.** Singlet fission: Optimal choice of mutual disposition of chromophores. Z. Havlas, P. Felkel, E. Buchanan, **J. Michl**

3:10 PHYS **305.** Dynamics of electronic excitations at organic-inorganic interfaces. **D. Kilin**, Y. Han, D. Vogel, A. Forde, B. Disrud, S.J. Jensen, W. Sapp, A.R. Erck

3:30 Intermission.

3:50 PHYS **306.** Conical intersections and non-radiative recombination in semiconductor nanocrystals. **B.G. Levine**, Y. Shu, B. Fales, W. Peng

4:20 PHYS **307.** Insights into the mechanism of photovoltaic action from photoacid-functionalized ion-exchange materials. **W.N. White**, C. Sanborn, D. Fabian, S. Ardo

4:40 PHYS **308.** Role of the protein in light-driven biological functions: A quantum chemical view. **B. Mennucci**

5:10 PHYS **309.** Understanding the quantum dynamics of photosynthetic energy transfer with realistic environment interactions. **P. Huo**, D. Coker, M. Lee

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Surface Chemistry, Sensors & Diagnostics

C. J. Murphy, *Organizer*

P. K. Jain, *Organizer, Presiding*

1:30 PHYS **310.** Plasmonic nanomaterials for ultrasensitive biosensing. **M. Stevens**

2:05 PHYS **311.** Dependence of the plasmonic properties of two silver nanocubes on their separation, relative orientation, refractive index of the substrate and propagation direction of the exciting light. **N. Hooshmand**

2:25 PHYS **312.** Controlling chirality of aluminum plasmonic architectures based on copper mask nanosphere template lithography. **J.S. Shumaker-Parry**

3:00 PHYS **313.** Understanding molecule-plasmon coupling in surface-enhanced femtosecond stimulated Raman scattering: Combined experimental-theoretical studies. **M.O. McAnally**, G.C. Schatz, R.P. Van Duyne

3:20 Intermission.

3:35 PHYS **314.** Commercialization of optically tailored plasmonic nanoparticles for diagnostic assays and therapeutics. **S. Oldenburg**, R.K. Baldwin, A.E. Saunders, J.M. Werle, R.T. Decker

4:10 PHYS **315.** Novel numerical method for electron energy-loss spectroscopy calculation: EELS-FDTD. **N. Large**, A. Manjavacas, E. Ringe, G.C. Schatz, S.X. Wang, P.J. Nordlander

4:30 PHYS **316.** SERS sensors for direct detection of environmental contaminants. **A.J. Haes**, T. Forbes, G. Lu

5:05 PHYS **317.** Plasmon-induced excited-state heterogeneous catalysis on surface-doped metallic nanoparticles. **J. Martirez**, E.A. Carter

Section F

Parc 55 San Francisco

Stockton

Dynamics & Structure of Molecular Fluids: Honoring the Work & Life of Branka Ladanyi

Water

N. E. Levinger, *Organizer*

A. T. Krummel, *Organizer, Presiding*

1:30 PHYS **318.** Mechanisms of electronic excited state relaxation in water clusters. **P.J. Rossky**

2:10 PHYS **319.** Withdrawn.

2:30 PHYS **320.** Solvation structure and photochemical dynamics of seeded molecular clusters. **G. Peslherbe**

3:10 Intermission.

3:30 PHYS **321.** Solvation dynamics revisited: An energy flux approach. **J.T. Hynes**, R. Rey

4:10 PHYS **322.** Connecting features of a water molecule with the anomalous properties of liquid water by comparing different water models in computer simulations. **T. Ichiye**

4:30 PHYS **323.** Hydration-shell vibrational spectroscopy of water-mediated interactions. **D. Ben-Amotz**

Section G

Parc 55 San Francisco

Fillmore

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Chemical Composition & Evolution of Comets 67P/CG: As Observed by the Rosetta Mission

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

L. Hornekaer, *Presiding*

1:30 PHYS **324.** Sugar derivatives in residues produced from the UV irradiation of astrophysical ice analogs. **M. Nuevo**, S.A. Sandford, J. Saunders, G. Cooper

2:15 PHYS **325.** Protonation and ionization of organic reactive molecules in low-density amorphous water ice. **W.W. Sander**, P. Costa, M.S. Gudipati

3:00 PHYS **326.** Radiation chemistry and redox reactions in icy molecular solids. **R.L. Hudson**, M. Loeffler

3:45 PHYS **327.** Electron induced chemistry in interstellar and cometary ices. **N.J. Mason**

4:30 PHYS **328.** Non-Ionizing UV (< 7 eV) photochemistry of cosmic ice analogs of ammonia. **H. Cumberbatch**, **A. Bao**, C. Arumainayagam

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

Sponsored by COMP, Cosponsored by PHYS

WEDNESDAY EVENING

Section A

Moscone Center

Hall D

PHYS Poster Session

J. E. Shea, *Organizer*

7:00 - 9:00

PHYS **329.** Study of the $O(^3P)$ initiated oxidation of 2-methylfuran via synchrotron multiplexed photoionization mass spectrometry. Y. Fathi, **K. Nwachuku**, G. Meloni

PHYS **330.** Photo-induced phase transitions of spin-crossover nanoparticles within the thermal hysteresis loop. **A.D. Mena**, D.A. Munteanu, R.M. van der Veen, T. Dixon, C.M. Gentle

PHYS **331.** Insight into the role of water in the photogeneration and properties of bifunctional quinone methides: A time-resolved spectroscopic study of a binol quinone methide. **L. Du**, X. Zhang, J. Xue, D.L. Phillips

PHYS **332.** Electronic dynamics in bulk GaAs induced by light with orbital angular momentum. **P. Navotnaya**, B.S. Rolczynski, G.S. Engel

PHYS **333.** Equivalency of the kinetic schemes: Mathematical formulation. **V.D. Dergachev**, A. Petrov, I. Dergachev, S.A. Varganov

PHYS **334.** Water, hydrogen-bonding networks, redox-active tyrosines, and proton coupled electron transfer reactions in the photosynthetic water oxidizing complex. **Z. Guo**, B.A. Barry

PHYS **335.** Withdrawn.

PHYS **336.** Accessing chiral information in macromolecules via time-resolved circular dichroism spectroscopy. **V. Stadnytskyi**, G. Orf, R.E. Blankenship, S. Savikhin

PHYS **337.** Methylglyoxal hydration state equilibrium at the air-water interface. **B. Gordon**, G. Lindquist, N.A. Valley, S. Wren, G.L. Richmond

PHYS **338.** Simulating transient x-ray absorption spectroscopy of photo-excited chemical dynamics in molecular systems. **S. Pemmaraju**, D. Prendergast

PHYS **339.** Characterization of the structure and dynamics of AOT reverse micelles in heavy alkanes. **I. Sitarik**, K. Obray, J. Diverdi

PHYS **340.** Exploring the role of asymetrically coordinated photoactive metal centers in photoinduced electron transfer reactions: A spectroscopic perspective. **B. Dietzek**

PHYS **341.** Chemistry of aerosolized room-temperature ionic liquids. **S. Chambreau**, G.L. Vaghjiani, D. Popolan-Vaida, S.R. Leone

PHYS **342.** Electron irradiation effects in icy regoliths: The PacMan anomalies on the icy Saturnian moons. **M.J. Schaible**, R.E. Johnson, L. Zhigilei

PHYS **343.** Effects of thermal broadening and photoluminescence in functionalized silicon nanocrystals. **D. Vogel**, D. Kilin

PHYS **344.** Undistorted fluorescence yield detected soft x-ray absorption spectroscopy: Direct detection of outer (3d->2p), inner (3s->2p) and inverse partial fluorescence yield using TES based spectrometers. **C. Titus**

PHYS **345.** Charge transfer dynamics at perovskite quantum dot and Spiro-MeOTAD interface. **D. Vogel**, D. Kilin

PHYS **346.** Withdrawn.

PHYS **347.** Binary mixtures consisting of glass-forming constituent and crystal-forming constituent: Density, rheology and phase transitions in poly(propylene glycol) – water system. **B.H. Milosavljevic**, S. Lovrinic

PHYS **348.** Simplifying calculations of IR and Raman spectra from DFT-based molecular dynamics simulations. **D.R. Galimberti**

PHYS **349.** Transient absorption spectroscopy with realtime TDDFT: Perovskites and Pauli bleaches. **J. Parkhill**

PHYS **350.** New mechanism for glass formation. **I.C. Sanchez**

PHYS **351.** Withdrawn.

PHYS **352.** Role of chloride ion in photosynthetic oxygen-evolution. **U. Brahmachari**, J.F. Gonthier, C. Sherrill, B.A. Barry

PHYS **353.** Theoretical ^{15}N isotropic chemical shift: Challenging the calculation of liquid state references. **F. Jolibois**, I. Gerber

PHYS **354.** Computational studies on chemistry of graphene surface. **B.Q. Pham**, M.S. Gordon

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PHYS **355.** Proposed two-dimensional topological insulator in SiTe. **Y. Ma**, T. Heine

PHYS **356.** Sunlight-Driven synthesis of oligomers from oxoacids in aqueous environments. **R. Rapf**, R. Perkins, V. Vaida

PHYS **357.** Ultrafast electron transfer in a model organic semiconductor: An experimental and theoretical examination. **V. Duong**, D. Nordlund, D. Prendergast, A. Ayzner

PHYS **358.** Optoelectronic structures of hybrid lead iodide perovskites probed by electron-rotor interaction. **J. Gong**, M. Yang, X. Ma, R.D. Schaller, G. Liu, L. Kong, Y. Yang, M.C. Beard, M. Lesslie, Y. Dai, B. Huang, K. Zhu, T. Xu

PHYS **359.** Spectroscopic and theoretical investigations of the intramolecular π-type hydrogen bonding in cyclic and bicyclic molecules. **J. Laane**, E.J. Ocola, A. Al-Saadi

PHYS **360.** Withdrawn.

PHYS **361.** Polarization anisotropy measurements for determining the orientation of guest molecules in a self-assembled bis-urea macrocycle host. **P. Kittikhunnatham**, B. Som, L.S. Shimizu, A. Greytak

PHYS **362.** Withdrawn.

PHYS **363.** Effects of exciton-delocalizing ligands on intraband relaxation in semiconductor nanocrystals. **M.S. Azzaro**, M.C. Babin, S.T. Roberts

PHYS **364.** Nonlinear interferometer for complex signal measurement. **M.J. Shultz**, J. Wang, P.J. Bisson, J. Marmolejos

PHYS **365.** Withdrawn.

PHYS **366.** Efficient geometry minimization and transition structure optimization using interpolated potential energy surfaces. **J. Zheng**, M.J. Frisch

PHYS **367.** Photon induced aerosol formation: Photochemically driven reactions of sulfur dioxide with water and organics. **J.A. Kroll**, V. Vaida

PHYS **368.** Angular dependence of ionization by short, intense pulses of linear and circularly polarized light simulated by time-dependent configuration interaction with an absorbing potential. **H.B. Schlegel**, P. Krause, P. Hoerner, Q. Liao, W. Li

PHYS **369.** Ultrafast transient absorption spectroscopy investigation of excited state dynamics of methyl ammonium lead bromide perovskite nanostructures. **H. Telfah**, J. Liu, A. Jamhawi, J. Strain, M. Teunis, R. Sardar

PHYS **370.** Modelling photodetachment processes in transition metal oxide clusters. **L.M. Thompson**, H.P. Hratchian

PHYS **371.** Lock and key bidentate binding of ligands on nanocrystals. **X. Li**, A. Fast, D. Fishman, Z. Huang, M. Tang

PHYS **372.** Multiple *cis* and *trans* conformations of caprylolactam and their role in deuterium isotope effect predictions in ^{13}C NMR. **E. Kleist**, B.S. Hudson

PHYS **373.** ϕ Photoreduction of $CHCl_3$ initiated by illumination of SPEEK/PVA and SPEEK/HCO_2^- system via a free radical mechanism. **M. Islam**

PHYS **374.** Withdrawn.

PHYS **375.** Tunable molecular separation by photoswitchable MOF membranes. **L. Heinke**

PHYS **376.** Nanoscale MoS_2towards emerging organic optoelectronics. A. Salam, **S. Pal**

PHYS **377.** Chiroptical investigation of sulfone-bridged heterohelicene. **A. Kim**, E. Mohammad, M. Vargas, A.G. Petrovic, B. Gliemann, M. Kivala

PHYS **378.** Withdrawn.

PHYS **379.** Tryptophan-to-tryptophan energy Transfer in UV-B photoreceptor UVR8. **X. Li**, D. Zhong

PHYS **380.** Withdrawn.

PHYS **381.** Withdrawn.

PHYS **382.** Accessing spatial heterogeneity in halide lead perovskite thin films with multimodal optical imaging. **Y. Ma**, M. Simpson, B. Doughty, S. Das, B. Yang, K. Xiao

PHYS **383.** Non-intrusive detection of polyatomic combustion intermediates via photoionization out of Rydberg states. **F. Rudakov**

PHYS **384.** Description of hydration water in protein (GFP) solution. **J. Nickels**, S. Perticaroli, G. Ehlers, C.B. Stanley, E. Mamontov, H.M. O'Neill, Q. Zhang, D. Myles, J. Katsaras

PHYS **385.** Raman studies of the photopolymerization of 1,4-diiodobuta-1,3-diene in crystalline urea inclusion compounds. **S. Dinca**, D.G. Allis, M.B. Sponsler, B.S. Hudson

PHYS **386.** Unequal hole and electron diffusion in lead bromide perovskites. **G. Elbaz**, D. Straus, O.E. Semonin, T. Hull, D. Paley, P. Kim, J.S. Owen, C.R. Kagan, X. Roy

PHYS **387.** First-principles calculations of the K-edge XANES spectra for aqueous Na^+ and for ion pairs of Ca^{2+} with either carbonate or bicarbonate. **M. Galib**, N. Govind, J. Fulton

PHYS **388.** Photoinduced charge transfer rates in light-harvesting carotenoid-porphyrin-C_{60} molecular triad. **X. Sun**, E. Geva

PHYS **389.** Inelastic neutron scattering analysis of tautomeric polymorphic crystals: The strange case of barbituric acid. **B.S. Hudson**, Y. Cheng

PHYS **390.** Exciton imaging in polycrystalline semiconducting organic thin films using optical resonance Imaging. **M.A. Allodi**, R.J. Mazukski, P.D. Dahlberg, H. Davis, J. Otto, G.S. Engel

PHYS **391.** Withdrawn.

PHYS **392.** High-Resolution infrared spectroscopy of carbon sulfur clusters. **J.B. Dudek**, J. Kozubal, T. Salomon, S. Fanghänel, S. Thorwirth

PHYS **393.** Electronic structure of iron-sulfur clusters revealed by 2p3d resonant inelastic x-ray scattering: Implications for biological nitrogen fixation. **B. Van Kuiken**, A. Hahn, S. DeBeer

PHYS **394.** Vacuum ultraviolet spectroscopy of the lowest-lying electronic state in sub-critical and supercritical water. **T.W. Marin**, I. Janik, D.M. Bartels, D. Chipman

PHYS **395.** Molecular simulations of Aβ-hIAPP cross-seeding assemblies on lipid membranes. **M. Zhang**, R. Hu, B. Ren, F. Yang, K. Chu, J. Zheng

PHYS **396.** Femtosecond stimulated Raman Spectroscopy of light harvesting complexes: Good vibrations in photosynthesis. **J. Artes Vivancos**, Y. Hontani, R. van Grondelle, J. Kennis

PHYS **397.** Synthesis and charge carrier dynamics of organolead bromide perovskite/graphitic carbon nitride nanoheterostructures for photocatalytic CO_2 reduction. **Y. Pu**

PHYS **398.** Partitioning, clustering, and hydrophobicity in mixtures of phospholipids and aromatics at water interfaces. **R. Perkins**, V. Vaida

PHYS **399.** Density fluctuations of carbon dioxide in cylindrical nanopore. **Y. Dai**, X. Xu, Y. Liu

PHYS **400.** From primordial soup to replicating DNA: Analyzing a proposed precursor of modern nucleotides. **K. Gochenour**, M.P. Callahan, K.E. Smith, D.K. Elliott, G.E. Lindberg

PHYS **401.** Investigation of electric potential induced by flowing water droplet on electrolyte-insulator-semiconductor structure. **J. Park**, Y. Yang, Y. Kim

PHYS **402.** Effect of salt and pH on the self-assembly of myristic acid. **B. Williamson**, R. Rapf, R. Perkins, V. Vaida

PHYS **403.** Confined phase separation of aqueous-organic nanodroplets. **F. Hrahsheh**, Y. Sani Wudil, G. Wilemski

PHYS **404.** Molecular properties of a light-gated cation channel from cryptophyta *Guillardia theta*. **Y. Yamauchi**, M. Konno, S. Ito, Y. Kato, S. Tsunoda, K. Inoue, H. Kandori

PHYS **405.** Triboelectric hydrogen gas detection using palladium functionalized surface. S. Shin, Y. Kwon, J. Jung, **J. Nah**

PHYS **406.** Asymmetric solvent-mediated electron-transfer chemical doping of graphene. **R.A. Dziatko**, **K. Harris**, M. Gibson, J. Karten, B. Janicek, A. Crowther

PHYS **407.** Nondestructive testing with second harmonic generation. **S.D. Smith**, S. Averett, J.E. Patterson

PHYS **408.** Nature of two diffuse interstellar bands revealed by electronic transitions in C_{60}^+. **S. Ahmadvand**, **A.O. Lykhin**, **S.A. Varganov**

PHYS **409.** Specific peptide-bond dissociation and effects of a phenyl group of some peptide model molecules. **C. Liu**, Y. Chiang, H. Lin

PHYS **410.** Vapor-liquid and liquid-liquid equilibria for a langmuir monolayer of pentadecanoic acid: A Monte Carlo study. **M.S. Minkara**, J. Siepmann

PHYS **411.** Withdrawn.

PHYS **412.** Excited-state dynamics of carotenoid dimers. **S.J. Doyle**, M.J. Tauber

PHYS **413.** Experimental and computational investigation of the competitive unimolecular reactions of CHF_2CHF_2 and CHF_2CF_3. C.A. Smith, G.L. Heard, **B.E. Holmes**

PHYS **414.** Transient grating spectroscopy of spheroidene and spheroidenone: The role of the carbonyl group in the excited state electronic and vibrational dynamics of carotenoids. S.D. Khosravi, M.M. Bishop, A.M. LaFountain, D. Busa, S. Suresh, D. Turner, G.N. Gibson, **H.A. Frank**, N. Berrah

PHYS **415.** ITC investigations on the dependence of temperature and osmometry on the structure and stability of the DNA I-motif. **T. Sutorius**

PHYS **416.** Theoretical investigation of RecA filaments search for DNA breaks. **M. Kochugaeva**, A. Shvets, A. Kolomeisky

PHYS **417.** Withdrawn.

PHYS **418.** Theoretical study on the reaction of silylidyne radical (SiH) with dimethylacetylene (CH_3CCCH_3). **Y. Lin**, M. Wu, B. Sun, A.H. Chang, R. Kaiser

PHYS **419.** Cl-initiated oxidation of propargylamine via synchrotron multiplexed photoionization mass spectrometry. **C. Price**

PHYS **420.** Withdrawn.

PHYS **421.** Investigation of glass structures using Raman spectroscopy. **V. Torres**, M.D. Sonntag

PHYS **422.** Ultrafast photoreleasing of the quinoline-derived phototrigger with sensitivity toward 2-photon excitation. **X. Lan**

PHYS **423.** Singlet/Triplet excited state mediated dehalogenation reactions of itraconazole in acetonitrile and aqueous solutions studied by time-resolved spectroscopy. **Z. Ruixue**, M. Li, L. Du, D.L. Phillips

PHYS **424.** Nanomorphology stabilization through the solvent additives and fixing agent interlayer for efficient organic and perovskite photovoltaic devices. **D. Wang**, W. Jang, S. Ahn, S. Park, J. Park

PHYS **425.** Quantum mechanical calculations of the effects of humidity on HNO_3 chemisorbed onto TiO_2. **C.J. Ostaszewski**, N.M. Stuart, J.G. Navea

PHYS **426.** Computational investigation of hydroperoxyl radical reacting with acetyl peroxy radical. **M.P. DeVault**, K.T. Kuwata

PHYS **427.** Computational study of hydride binding to the active site of lactate racemase. **R.C. Mauban**, S.A. Varganov

PHYS **428.** Temperature dependence of the hydrated electron's excited-state relaxation: Distinguishing cavity and non-cavity models. **C. Zho**, E.P. Farr, W.J. Glover, B.J. Schwartz

PHYS **429.** Excited state proton transfer kinetics of aminonaphthols in aqueous reverse micelles. **A.P. Poblete**, K. Takematsu

PHYS **430.** Photochemical reactivity of oxoacids in aqueous solution as a function of pH. **M.R. Dooley**, **R. Rapf**, R. Perkins, V. Vaida

PHYS **431.** Prevention of fibrillation of the amyloid-β (25-35) peptide by graphene oxide. **S. Bag**, S. DasGupta, S. Dasgupta

PHYS **432.** FTIR analysis of internal water molecules of a light-driven sodium pump KR2. **S. Tomida**, S. Ito, K. Inoue, H. Kandori

PHYS **433.** Kinetic modeling of the atmospheric oxidation pathways of dimethyl disulfide and dimethyl sulfide. **J.A. Berlanga**

PHYS **434.** Withdrawn.

PHYS **435.** Photoaddition of methanol to the stilbenes: Involvement of a common twisted intermediate. **S. Gupta**, D. Boose, J. Saltiel

PHYS **436.** Utilizing electron spin echo envelope modulation to distinguish between the local secondary structures of an α-helix and an amphipathic 310-helical peptide. **S. Rafferty**

PHYS **437.** Hybrid nano-biosystems: An investigation of the impact of quantum dots on the bacteriorhodopsin photocycle. **T.J. Wax**, J.A. Greco, S. Chen, J. Zhao, R.R. Birge

PHYS **438.** Thermal study of the decomposition of (HTPB) hybrid rocket fuel in the presence of azo-tetrazolate based high nitrogen content high energy materials. **M. Yousef**, K. Hudson

PHYS **439.** Metal free, redox-active, viologen-based, Deep Eutectic Solvents (DES). **L.N. Matsushima**, J.C. Goeltz

PHYS **440.** Optical transitions in bulk semiconductors induced by light carrying orbital angular momentum. **P. Navotnaya**, B.S. Rolczynski, G.S. Engel

PHYS **441.** Core-shell MoS_2/CdS nanorods with extraordinary high photocatalytic activity for hydrogen production under visible-light. **Z. Yan**

PHYS **442.** Developing and implementing methods for Markov state model construction and conformational sampling to extract the kinetics of protein-protein interactions. **Z. He**

PHYS **443.** Decomposition of contributions from core-levels exhibiting spin-orbit splitting in XUV core-level spectroscopy. **H. Chang**, M.W. Zuerch, P. Kraus, C. Kaplan, L.J. Borja, S. Cushing, D.M. Neumark, S.R. Leone

PHYS **444.** Withdrawn.

PHYS **445.** Unusual pattern formation in the cadmium hydroxide system. **B. Bohner**, Á. Tóth, D. Horvath

PHYS **446.** Photofragmentation dynamics of tetranitromethane. **Y. Han**, B. Rasulev, D. Kilin

PHYS **447.** Can zwitterionic cyclic polymers show aggregation in solution? **P. Du**, A. Li, X. Li, R. Kumar, D. Zhang

PHYS **448.** Molecular dynamics of reaction between hydrogen peroxide and zigzag carbon nanotube. **B. Disrud**, D. Kilin

PHYS **449.** Photophysical studies of nitro substituted porphyrinoids. **A. Aggarwal**, **C. Farley**, C.M. Drain

PHYS **450.** First-principles calculations of electron transfer rates. **S. Chaudhuri**, S. Hedström, D.D. Mendez, H.P. Hendrickson, K. Jung, V.S. Batista

PHYS **451.** Proton diffusion from pH gradients on litmus paper. **S. Ostresh**

PHYS **452.** Estimating the redox potentials of organic dyes in dichloromethane. **F.A. Rodriguez Ortiz**, D. Méndez-Hernández

PHYS **453.** Photo-conductivity measurements of water-rich ices at cryogenic temperatures. **D. Marchione**, R. Yang, M.S. Gudipati

PHYS **454.** Solution behavior and self-assembly of nanoscale macroions into "Blackberry" structure through charge mediated attractions. **S. Eghtesadi**, P. Yin, D. Li, F. Haso, Y. Gao, T. Liu

PHYS **455.** Analyzing phosphorylation of prebiotic molecules by schreibersite with polarization-modulation: Infrared reflection-absorption spectroscopy. **K. Slavicinska**, T.J. Beckman, H.L. Abbott-Lyon

PHYS **456.** Spectroscopic characterization of the physical and photo-physical properties of pewly peveloped platinum pincer complexes. **S.A. Autry**, M. Zhang, V. Dixit, T.K. Hollis, C.E. Webster, N. Hammer

PHYS **457.** Studies of nanoparticle impact dynamics with the aerosol impact spectrometer. **M.E. Miller**, B.D. Adamson, R.E. Continetti

PHYS **458.** Synchrotron multiplexed photoionization mass spectrometry of Cl-initiated oxidation of tetrahydropyrane (THP) at 298, 550, and 650 K. **A. Otten**

PHYS **459.** Charge carrier dynamics in highly luminescent cesium lead halide nanocrystals. **N. Gibson**

PHYS **460.** Photoionization and photodissocation of xylyl (methylbenzyl) bromide radicals using VUV synchrotron radiation. **Y. Fathi**, G. Meloni, P. Hemberger

PHYS **461.** Solvent thermodynamic driving force controls stacking interactions between polyaromatics. A. Rury, C.E. Ferry, **J.R. Hunt**, M. Lee, D. Mondal, S. O'Connell, E.N. Phan, Z. Peng, P. Pokhilko, D. Sylvinson, Y. Zhou, C.H. Mak

PHYS **462.** Withdrawn.

PHYS **463.** Si-SiO_x-Al_2O_3 Composite with carbon coating as an anode material for Li-ion batteries. **K. Kim**, J. Kim

PHYS **464.** Non-Thermal plasma for the heterogeneous chemistry of chemisorbed volatile compounds with free-radicals. **C. Bennett-Caso**, J.R. Borgatta, J.G. Navea

PHYS **465.** Excited-state investigation of the ultrafast electrocyclization reaction for a molecular photochromic switch. **C. Jones**, V.A. Spata, S. Matsika

PHYS **466.** PhotochemCAD 3. digital database of >1000 absorption and fluorescence spectra of diverse natural and synthetic tetrapyrrole macrocycles. **M. Taniguchi**, H. Du, J.S. Lindsey

PHYS **467.** Nonadiabatic dynamics in the formation of the elusive disilavinylidene molecule (H_2SiSi). C. Kang-Heng, **L. Lin**, A.H. Chang, R. Kaiser

PHYS **468.** Nonadiabatic dynamics of $Si(^3P) + Si_2H_6$ reaction. B. Sun, **C. Jimmy**

PHYS **469.** In-situ x-ray spectroscopy study of electrodeposited Ni-Fe hydroxide catalysts for electrochemical oxygen evolution reaction. **K. Nie**

PHYS **470.** Two-Dimensional electronic spectroscopy of BODIPY dye derivatives: Characterizing photophysics and solvent dependence. **Y. Lee**, S. Das, R.M. Malamakal, S. Meloni, D.M. Chenoweth, J.M. Anna

PHYS **471.** MRCI study of the ground state and low-lying states of Si_2H. **D. Corey**, J. Song

PHYS **472.** Apparent molar volumes and isentropic compressions of cyclic ethers in aqueous solutions from 288.15 K to 313.15 K at atmospheric pressure. **L. Brown**, P. Bernal

PHYS **473.** Electrochemical impedance spectroscopy of bipolar membranes for water and CO_2 electrolysis. **Z. Yan**, L. Zhu, C.C. Li, M. Hickner, T. Mallouk

PHYS **474.** Excited-State proton transfer in aminonaphthols. **M. Groves**, H.E. Rudel, K. Takematsu

PHYS **475.** Experimental determination of the aqueous redox potentials of environmentally relevant organic pollutants via high-speed cyclic voltammetry. **M. Paul**, D. Ruuska, S.N. Eustis

PHYS **476.** Brillouin spectroscopy of bamboo fibers. **D. Williams**, N. Rahbar, K.J. Koski

PHYS **477.** Anisotropic optical response from asymmetrical assembly of gold-silica-quantum dot nanostructure. **Y. Luo**

PHYS **478.** Enhanced sampling method with hybrid non-equilibrium molecular dynamics/Monte Carlo. **D. Suh**, C. Chipot, B. Roux

PHYS **479.** Novel approach to investigate the single molecule photophysics of bare CdSe quantum dots. **B. Mehlenbacher**, J.J. Peterson

PHYS **480.** Synthesis of iron series phosphate micro-nano-materials and their potential applications for electrochemical energy storage. **H. Xue**, Y. Yan, H. Pang

PHYS **481.** New inorganic pH indicator based on ferricyanide intercalated zinc-aluminum layered double hydroxide. **N.A. Ibrahim**, A. Chaparadza

PHYS **482.** Many-Body expansion combined with neural networks. **K. Yao**, J. Herr, J. Parkhill

PHYS **483.** Albumin based nanoparticles as a delivery vehicle for flavonoids and their anticancer activity. **P. Ghosh**, S. Dasgupta

PHYS **484.** Stability of bovine serum albumin solutions in presence of salts: A calorimetric and solubility study. T. Janc, V. Vlachy, **M. Luksic**

PHYS **485.** Noninvasive detection of aluminum sensitization using SHG. **A. Farnsworth**, S. Averett, K. Rellaford, S.D. Smith, J.E. Patterson

PHYS **486.** Feasibility of *in situ* magnetic resonance imaging of semi-industrial chemical reactors at milli-Tesla magnetic fields. **D. Barskiy**

PHYS **487.** Influence of pH on the photochromic reaction dynamics of phenylamine-substituted diarylethene derivatives. **S. Mahvidi**, C.J. Otolski, Y. Yokoyama, F. Nourmohammadian, C.G. Elles

PHYS **488.** Ultrafast energy relaxation dynamics and wave-packet motion in Pt(II) bimetallic complexes. P. Kim, S. Brown-Xu, A. Chakraborty, **F.N. Castellano**, **L.X. Chen**

PHYS **489.** Investigation on pyrolsis of jet propellant 8. **D. Belisario-Lara**, A.M. Mebel

PHYS **490.** Post-Marcus charge transfer dynamics via the generalized quantum master equation. **E. Mulvihill**, E. Geva, A. Schubert, X. Sun, A. Kananenka

PHYS **491.** Withdrawn.

PHYS **492.** Molecule-nanocrystal photon upconversion sensitized by CdSe/CdS core-shell nanocrystals. **Z. Huang**, M.L. Tang

PHYS **493.** Bath gas and pressure dependence of the anomalous isotopic composition of ozone. **A.H. Kazez**, K.A. Boering

PHYS **494.** Jet-cooled high resolution infrared spectroscopy of small van der Waals SF_6 clusters. **A. Turner**, Y. Berger, V. Boudon, L. Bruel, M. Gaveau, M. Mons, A. Potapov, P. Asselin

PHYS **495.** Withdrawn.

PHYS **496.** Ultrafast photophysics of plasmonic aluminum nanoparticles. **K. Smith**, Y. Cheng, E. Arinze, S. Thon, A.E. Bragg

PHYS **497.** Modeling of hydrodynamic interactions in biological systems. **M. Dlugosz**

PHYS **498.** Optimization of energy transfer in DNA-dye excitonic circuits. **W. Bricker**, J. Banal, R. Veneziano, K. Pan, M. Bathe

PHYS **499.** Theoretical investigation of vibrational frequency shifts as probes of charge transfer in organic systems. **K. Williams**, E. Geva

PHYS **500.** Theoretical study on photoluminescence properties of double salts of silver and gold complexes. **S. Chen**, B. Sun, A.H. Chang, I.J. Lin

PHYS **501.** Computations of the hyperpolarizability of nonlinear optical chromophores aggregates. **X.A. Sosa Vazquez**, J. Maat, C. Isborn

PHYS **502.** Surface-Enhanced Raman scattering analysis of DNA modifications in the presence of carboplatin. **N. Mirsaleh-Kohan**, S. Khan, M. Torres, M. Duplanty, P. Hall, M. Garrett

PHYS **503.** Water solubilization of $CuInS_2$/ZnS QDs and bioconjugation to fibroblast growth factor studied by FRET. **C. Robinson**, M. Mohale, A. Nguyen, C.D. Heyes

PHYS **504.** Nonradiative relaxation in real-time electronic dynamics OSCF2: Organolead triiodide perovskite. **T.S. Nguyen**, J. Parkhill

PHYS **505.** Characterization of α-hemolysin conformational changes with two-dimensional infrared spectroscopy. **C.T. Kuhs**, A.T. Krummel

PHYS **506.** Time resolved resonance Raman spectroscopic and laser flash photolysis studies on typical significant stocks-shifted large π system. **L. Song-Bo**, M. Li, Z. Ruixue, D.L. Phillips

PHYS **507.** Withdrawn.

PHYS **508.** Anomalies of ice Ih in second-order many-body perturbation theory. **M. Salim**, S. Hirata

PHYS **509.** Withdrawn.

PHYS **510.** Microwave spectroscopy of 3,3,3-trifluoro-2-(trifluoromethyl)propanoic acid-formic acid complex. J. Thomas, **M.J. Carrillo**, A. Serrato, W. Jaeger, Y. Xu, W. Lin

PHYS **511.** Ultrafast extreme-ultraviolet reflection spectroscopy of electro-phonon dynamics in Germanium. **C. Kaplan**, P. Kraus, L.J. Borja, M.W. Zuerch, H. Chang, M.F. Jager, S. Cushing, D.M. Neumark, S.R. Leone

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PHYS **512.** Photoionization cross sections of three propargylic fuels. **M. Winfough**, G. Meloni

PHYS **513.** Simulating the chemistry of ionizing radiation in solids. **C.N. Shingledecker**, E. Herbst

PHYS **514.** Synthesis and photophysical characterization of bipyridyl hybrid oligomers: Examining mixed furan-thiophene systems using spectroscopy and DFT methods. **A.E. Steen**, S. Nguyen, T.L. Ellington, G.S. Tschumper, D.L. Watkins, N. Hammer

PHYS **515.** Modeling protein organization in thylakoid membrane stacks via a lattice gas model. **A. Rosnik**, P. Geissler

PHYS **516.** Quantum control of Yukawa interaction at nucleus. **Q. Wang**

PHYS **517.** Withdrawn.

PHYS **518.** Structural trends and reactivity of first-row transition metal cation-acetylene complexes revealed by probing their C-H stretching fundamentals. **A.D. Brathwaite**, S.A. Ferguson, T.B. Ward, R.S. Walters, M.A. Duncan

PHYS **519.** Nonadiabatic dynamics of $C(^3P) + SiH_4$ reaction. **A.H. Chang**

PHYS **520.** Preferential solvation of iodide anion in aqueous binary liquid mixtures. **Y. Al Hussain**, B.H. Milosavljevic

PHYS **521.** Rotational spectroscopic and theoretical studies of the perfluorobutyric acid--formic acid complex. J. Thomas, **A. Serrato**, M.J. Carrillo, W. Lin, W. Jaeger, Y. Xu

PHYS **522.** Molecular geometry and conformation analysis of the monomer and monohydrate of 4,4,4-trifluorobutyric acid. **A. Treviño**, W. Lin

PHYS **523.** Spatially extended active site: How distal residues contribute to catalysis in human phosphoglucose isomerase. **S.C. Begay**, P.J. Beuning, M.J. Ondrechen

PHYS **524.** Electronic structure and RRKM calculations on the reaction $CH_3OH_2^+ + CH_3OH$. **M. Rosi**, S. Falcinelli, N. Balucani, N. Faginas-Lago, C. Ceccarelli, D. Skouteris

PHYS **525.** Photophysical characterization of free-base triphenylcorrole reduced and oxidized tautomers. **G.N. Calvillo**, **C. Reed**, F. Kohl, S. Klein, A. Loogman, S. Lupercio, E.A. Alemán

PHYS **526.** Enthalpy relaxation below T_g in low molecular weight poly(dimethylsiloxane). **D. Eason**, A.D. Schwab

PHYS **527.** Role of ion-specific effects in DNA/ionene complexation. M. Seručnik, B. Zener, **B. Hribar Lee**

PHYS **528.** Effects of the anion nature of cationic polymethine dyes on the spectral-luminescent and photovoltaic properties of polymer-based photoconductive composites. A.A. Ishchenko, G. Bulavko, **N. Barashkov**, **T. Sakhno**

PHYS **529.** Investigation of relationship between the rate of converting leuco form of Indigo Carmine in its colored form and oxygen permeability of polymer films. **N. Barashkov**, I. Irgibayeva, **T. Sakhno**

PHYS **530.** Novel approaches to the development of biosensor by using systems of formulation and analytical techniques. **G. Ren**, Y. Lo, E.J. Parish, **H. Honda**, T. Wei

PHYS **531.** Tuning the structure and photophysics of a fluorous phthalocyanine platform. **C.M. Drain**, C. Farley

PHYS **532.** Using isothermal titration calorimetry to investigate dicationic alkylammonium bromide Gemini surfactants. M.L. McKim, B.K. Rich, P. Okoroji-Ohabor, S.J. Bachofer, **R.D. Sheardy**

PHYS **533.** Linking pH, temperature, ionic strength and conformation for the DNA i-motif. **T. Nguyen**, C. Fraire, A. Fernandes, M. Choi, **R.D. Sheardy**

PHYS **534.** Uncertainty and sensitivity analysis of the Marcus electron transfer rate model. **E.J. Alvarado**, D.D. Mendez, E.J. Morales-Butler, M. Cruz-Aponte

PHYS **535.** Tensor structured coupled cluster method. **R. Schutski**, G.E. Scuseria

PHYS **536.** Evaluation of VLE data from the TraPPE Force Field. **B.L. Eggimann**

PHYS **537.** DNA mutation and fluorescent label effects in surface-bound 25mer microarrays: Molecular simulation of bright mismatches. B. Rivard, **J.M. Stubbs**

PHYS **538.** Photochemical activity of layered potassium niobate in the redox processes. V. Shvalagin, G. Grodzyuk, N. Andryushina, V. Granchak, M. Skoryk, **T. Sakhno**, **N. Barashkov**

PHYS **539.** Investigation of the mechanism of fullerene and carbon nanotube formation by molecular dynamics simulation. **B. Amofah**, T.J. Fuhrer

PHYS **540.** Quantum chemical studies of ether formation with peroxide reagents. **K.T. Kuwata**, T. Truttmann

PHYS **541.** Investigation of organic radicals and intermediates via high-resolution infrared spectroscopy. **M.D. Schuder**, A. Kortyna, D.J. Nesbitt

THURSDAY MORNING

Section B

Parc 55 San Francisco

Powell

Spectroscopy of Complex Systems

Effects of Nanoconfinement & Local Asymmetry on Dynamics & Chemistry: Interfaces

J. Dawlaty, *Organizer*

A. V. Benderskii, *Organizer, Presiding*

8:00 PHYS **542.** Sum frequency generation spectra from density functional theory. **V.S. Batista**

8:40 PHYS **543.** Measuring orientation heterogeneity of heterogeneous catalysts using HD 2D SFG spectroscopy. **W. Xiong**, Z. Li, J. Wang, Y. Li

9:00 PHYS **544.** Heterodyne-detected sum frequency generation spectroscopy of aqueous interfaces. **S. Yamaguchi**

9:40 Intermission.

10:00 PHYS **545.** Chiral water structures in biological systems. M. McDermott, H. Vanselous, S. Sanders, **P.B. Petersen**

10:40 PHYS **546.** Water bending vibration: A closer look at the flip-flop of water molecules at charged interfaces. **C. Dutta**, M. Mammetkuliyev, A.V. Benderskii

11:00 PHYS **547.** Probing the surfaces of CdSe quantum dots using sum frequency generation. **B.R. Watson**, B. Doughty, T.R. Calhoun

11:20 PHYS **548.** Vibrational sum-frequency scattering spectroscopy reveals the detailed surface chemistry of biomaterials in aqueous solutions. **P.K. Johansson**, L. Schmüser, Y. Wang, D.G. Castner

11:40 PHYS **549.** Understanding catalytic selectivity via the absolute molecular orientation of adsorbed interfacial molecules. **B. Doughty**, S. Goverapet Srinivasan, S. Bryantsev, D. Lee, H. Lee, D.R. Salahub, Y. Ma, D.A. Lutterman

Section C

Parc 55 San Francisco

Hearst

Sunlight-Driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

Exciton Photodynamics: Hard Materials

D. S. Larsen, M. Olivucci, *Organizers*

K. Glusac, *Organizer, Presiding*

8:00 PHYS **550.** Photoexcited carriers recombination and trapping in spherical vs faceted TiO2 nanoparticles. **C. Di Valentin**, G. Fazio, L. Ferrighi, D. Selli

8:30 PHYS **551.** Withdrawn.

8:50 PHYS **552.** Withdrawn.

9:20 PHYS **553.** Ultrafast transient absorption spectroscopy investigation of photoinduced dynamics in donor-acceptor core-shell nanostructures for organic photovoltaics. **J. Strain**, T.M. Abeywickrama, H.P. Rathnayake, J. Liu

9:40 Intermission.

10:00 PHYS **554.** Role of interfaces on hybrid perovskite photocarrier dynamics. **D.S. Ginger**

10:30 PHYS **555.** Bulk carrier dynamics in nanocrystalline organo-halide perovskites through surface passivation. R. Stewart, **J.B. Asbury**

11:00 PHYS **556.** Direct charge transfer at organic semiconductor/metal interfaces. **W. Xiong**, Y. Li, B. Xiang

11:20 PHYS **557.** Excitation dynamics in nanoscale materials for solar energy harvesting: Time-domain ab initio studies. **O.V. Prezhdo**

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Solutions to the Energy Problem

C. J. Murphy, *Organizer*

P. K. Jain, *Organizer, Presiding*

8:00 PHYS **558.** Aluminum plasmonics: From new chemistry to new applications. **N.J. Halas**

8:35 PHYS **559.** Imaging acoustic-to-plasmonic vibrational dynamics with ultrafast electron microscopy. **D.J. Flannigan**, V.E. Ferry, D.T. Valley

8:55 PHYS **560.** Shine down - cut the cord. T. Tumkur, X. Yang, W. Wang, B. Jiang, X. Zhang, Y. Wei, S. Bahauddin, H. Robatjazi, B. Cerjan, C. Doiron, X. Liu, P. Wray, L. Vayssieres, N.J. Halas, P.J. Nordlander, **I. Thomann**

9:30 PHYS **561.** Impact of dopant choice on the optical response and near-field enhancement of doped indium oxide nanocrystals. **R.W. Johns**, D.J. Milliron

9:50 Intermission.

10:05 PHYS **562.** Withdrawn.

10:40 PHYS **563.** Strong coupling of localised surface plasmons to light-harvesting complexes from bacteria and plants. A. Tsargorodska, M. Cartron, G. Kodali, L. Dutton, C. Hunter, P. Torma, **G.J. Leggett**

11:00 PHYS **564.** Device applications of metafilms. **M. Brongersma**

11:35 PHYS **565.** Gas phase catalytic cycle of hydrogen production from water using small Mo-oxide cluster anions. **M. Ray**, A. Saha, C. Jarrold, K. Raghavachari

Section F

Parc 55 San Francisco

Stockton

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices & Catalysis on Interstellar Grains

Radiation Chemistry of Europa's Surface

R. Kaiser, *Organizer*

M. S. Gudipati, *Organizer, Presiding*

L. M. Ziurys, *Presiding*

8:00 PHYS **566.** Coupled surface-atmosphere chemical production of oxidants in the solar system. **S.K. Atreya**

8:45 PHYS **567.** Carbon dioxide chemistry at low temperatures. **R. Hodyss**, S. Piao, M.L. Cable, M.J. Malaska

9:30 PHYS **568.** Primary phosphorus sources within extraterrestrial ices. **M.A. Pasek**

10:15 PHYS **569.** Investigating the formation of alkylphosphonic acids in phosphine ices. **A.M. Turner**, R. Kaiser

10:45 PHYS **570.** Synthesis of di-depsipeptides under possible solar system environments. **E.T. Parker**, J.G. Forsythe, F.M. Fernandez

11:15 PHYS **571.** Infrared matrix isolation spectroscopy of photochemical products of acetylene and nitrogen in argon matrices. **B.T. Genest**, P.D. Cooper

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Inhibition & Therapeutic Applications of Allosteric Mechanisms

Sponsored by COMP, Cosponsored by PHYS

Engaging Students in Physical Chemistry

Sponsored by CHED, Cosponsored by PHYS

THURSDAY AFTERNOON

Section D

Parc 55 San Francisco

Divisadero

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals to Societal Impacts

Solutions for Medicine

P. K. Jain, *Organizer*

C. J. Murphy, *Organizer, Presiding*

1:30 PHYS **572.** Photothermal therapy of cancer in cells and in different animals using gold nano-rods: A progress report. **M.A. El-Sayed**

2:05 PHYS **573.** Single-Molecule super-resolution study of distance-dependent plasmonic fluorescence enhancement and emission mislocalization. **B. Fu**, J.S. Biteen

2:25 PHYS **574.** Plasmonic biosensors for resource-limited settings. **S. Singamaneni**

3:00 PHYS **575.** Nonlinear and ultrafast spectroscopy of gold-silver-gold core-shell-shell nanoparticles. **L.H. Haber**, T.E. Karam, R.R. Kumal, H. Smith, R.A. Khoury, B. Kruger, J. Ranasinghe, Z. Zhang

3:20 Intermission.

3:35 PHYS **576.** Manipulating light-matter interactions in bioprogrammable crystals. **C.A. Mirkin**

4:10 PHYS **577.** Plasmonics at the cluster limit: Dielectric sensing with DNA-stabilized silver clusters. **S.M. Copp**, D. Schultz, S. Swasey, A. Faris, E. Gwinn

4:30 PHYS **578.** DNA-Encapsulated silver cluster chromophores. **J.T. Petty**, R. Dickson, T. Yeh

Allosteric Interactions & Regulation of Complex Biomolecular Systems: From Proteins to Cell Signaling

Mechanisms & Molecular Simulations

Sponsored by COMP, Cosponsored by PHYS

POLY

Division of Polymer Chemistry

C. Lipscomb, *T. White and T. Epps, Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Materials, Devices, and Switches (see *ORGN,* Tue, Wed, Thu)

Peptides, Proteins & Amino Acids (see *ORGN,* Tue, Wed)

Polymers under Deformation (see *PMSE,* Tue, Wed)

SOCIAL EVENTS:

Reception, 5:00 PM: Tue

Reception, 5:30 PM: Wed

Breakfast, 7:30 AM: Tue

Luncheon, 12:00 PM: Sun

SUNDAY MORNING

Section A

Moscone Center

120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

A. M. Alb, P. S. Majumdar, *Presiding*

8:00 POLY **1.** Design of experiments based approach to investigate the adhesion of latex paints over alkyd surfaces. **P.S. Majumdar**, J. Sweeney, C. Kozak, S.A. Carpenter, S. Eberly, W. Howell, L.C. Fioravanti, A.M. Piwowar

8:20 POLY **2.** Measurement and control of migrating species on waterborne coatings surfaces. **J. Bohling**, J. Gallagher, A. Gong, K. David, B. Cooper

8:40 POLY **3.** Mussel inspired coatings based on tannic acid and polyamines. **I. Yilgor**, E. Yilgor, C. Kosak

9:00 POLY **4.** Withdrawn.

9:20 POLY **5.** Macromolecular characterization of biopolymers as alternative depressants for iron ore flotation. **A.M. Alb**

9:40 POLY **6.** Shape memory polymers from amino acid-based poly(ester urea)s. **G.I. Peterson**, E.P. Childers, J. Yu, H. Li, A. Dobrynin, M. Becker

10:00 POLY **7.** Withdrawn.

10:20 POLY **8.** Effect of monomer sequence on the properties of hyperbranched copolymers. **Y. Shi**, H. Gao

10:40 POLY **9.** Synthesis and characterization of new high temperature multigraft copolymer superelastomer: Polyisoprene-graft-polybenzofulvene. **H. Wang**, W. Wang, W. Lu, X. Lu, N. Kang, J.W. Mays

11:00 POLY **10.** Tunable photonic nanocomposite film formed by gelation of self-assembled block copolymer. **Y. Huang**, Y. Zheng, J. Pribyl, B.C. Benicewicz

11:20 POLY **11.** Topology transformation of rotaxane-linked star/linear ABC terpolymer: Synthesis and characterization. **H. Sato**, D. Aoki, T. Takata

11:40 POLY **12.** Visualizing randomness: Synthesis and imaging of statistical and segmented colloidal copolymers. **N.G. Pavlopoulos**, J. Pyun

Section B

Moscone Center

121

Next Generation Smart Materials

Cosponsored by MPPG‡

Y. C. Simon, *Organizer*

E. B. Berda, J. Foster, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **13.** Antisense gene regulation with non-cationic polymer carriers. **K. Zhang**

8:35 POLY **14.** Sulfur-free RAFT, sequence-controlled methacrylic multiblockcopolymers via emulsion polymerization. **D.M. Haddleton**, A. Anastasaki, N. Engelis, V. Nikolaou, G. Nurumbetov

9:05 POLY **15.** Precision functional polyethylene-based polymers via acyclic Diene Metathesis (ADMET). **K.B. Wagener**, M.H. Bell, H. Li, T.W. Gaines

9:35 Intermission.

9:45 POLY **16.** One-pot synthesis of responsive polymers with highly branched structures. **H. Gao**, Y. Shi, X. Cao

10:15 POLY **17.** Shape memory in self-healing polymers: Synchronized physico-chemical events. Y. Yang, C.C. Hornat, **M.W. Urban**

10:45 POLY **18.** Host-guest chemistry to control polymeric architecture and conformation. **H.W. Gibson**, T. Price, H. Wessels, Z. Bear

Section C

Moscone Center

122

Polymeric Materials for Performance & Sustainability

Biobased Polymers

Cosponsored by MPPG‡

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

J. M. McCollum, *Presiding*

8:00 Introductory Remarks.

8:10 POLY **19.** Molecular dynamics simulation of cellulose nanofibrils used to modify polymer gels. **Y. Sliozberg**, S. Coleman, H. Dong, J. Snyder, A. West, T. Chantawansri

8:40 POLY **20.** Mechanophore activation at the crosslinked epoxy-nanocellulose interface: Insight from density functional theory and molecular dynamics simulations. **K.S. Khare**, F.R. Phelan

9:10 POLY **21.** Ductile polyacrylonitrile fibers with high cellulose nanocrystals loading. **H. Chang**, J. Luo, H.c. Liu, A. Bakhtiary Davijani, P. Wang, G. Lolov, R. Dwyer, S. Kumar

9:30 Intermission.

9:45 POLY **22.** New and unexpected properties from polycyanurate networks prepared from biobased monomers. **A.J. Guenthner**, B.G. Harvey, A.P. Chafin, M.C. Davis, J. Zavala, K. Lamison, J. Reams, M.D. Ford, K. Ghiassi, T.J. Groshens, J.M. Mabry

10:15 POLY **23.** Styrene-free soybean oil-based thermosets and their natural fiber composites. **W. Liu**, R. Qiu

10:35 POLY **24.** Synthesis and properties of new cross-linked bio-based aliphatic polycarbonates. **P. Durand**

10:55 POLY **25.** Transient networking in glucarodilactone-containing polyesters. **L.M. Lillie**, W.B. Tolman, T.M. Reineke

Section D

Moscone Center

123

Separation of Macromolecules & Particulates

Cosponsored by ANYL, COLL and PMSE

Financially supported by PSS Polymer Standards Service GmbH, The Dow Chemical Company, Tosoh Bioscience LLC, Wyatt Technology

S. V. Orski, Y. Wang, *Organizers*

W. Gao, X. M. Liu, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **26.** Theoretical perspective on the separation mechanism of complex polymers by interaction chromatography. **Y. Wang**

8:45 POLY **27.** Polymer microstructure analysis by HPLC. **D. Lee**, S. Qiu, J. Munro, C. Li Pi Shan, T. Huang, R. Cong

9:15 POLY **28.** Separation and characterization of living and dead chains in polystyrene synthesized by ATRP. **T. Chang**

9:45 Intermission.

9:55 POLY **29.** Understanding of aqueous oligomers formed during emulsion polymerization and their interfacial behavior via LC-MS. **T. Zhang**, B. McCulloch, W. Gao, R. Even

10:25 POLY **30.** Copolymer structure elucidation by multidimensional techniques with focus on UPLC x ESI-TOF-MS. **J. Falkenhagen**

10:55 POLY **31.** Application of different chromatographic techniques to characterize chemical and molar mass heterogeneity in graft copolymers. R. Leinweber, P. Montag, J. Preis, **W. Radke**

11:25 POLY **32.** Large-scale separation and purification of block copolymers via selective and competitive adsorption on silica. **C.Y. Ryu**

Section E

Moscone Center

124

Incorporating Polymer Science into the Classroom

Undergraduate Curriculum

Cosponsored by CHED, MPPG‡ and PMSE

K. A. Cavicchi, S. E. Morgan, *Organizers*, *Presiding*

8:00 POLY **33.** Green synthesis of renewable triblock polymers in the organic chemistry laboratory: Not your typical white solid. **J.E. Wissinger**

8:25 POLY **34.** Undergraduate polymer synthesis developed for lecture and laboratory experiments. **P.J. Costanzo**

8:50 POLY **35.** Integration of polymerization kinetics in polymer, physical chemistry, and chemical engineering courses. **A. Guymon**

9:15 Intermission.

9:30 POLY **36.** Polymer physical structure labs at Allegheny College. **R.M. Van Horn**

‡*Cooperative Cosponsorship*

9:55 POLY **37.** Studying the thermomechanical properties of copolymers to develop laboratory, theoretical, and communication skills essential to a successful research career. **S.A. Sydlik**, W. Koshut, Z. Wright, Z. Smith

10:20 POLY **38.** Polymeric materials in the beginning organic chemistry course. **B.A. Howell**

Section F

Moscone Center

125

Polymer Applications & Characterization in the Biomedical Industry

X. M. Liu, J. Slager, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **39.** Nitric oxide-releasing hyperbranched polykanamycin as an oral therapeutic. **L. Yang**, X. Wang, D.J. Suchyta, M. Schoenfisch

8:35 POLY **40.** Withdrawn.

9:05 POLY **41.** Universal multifunctional coating of biominerals based on salivary acquired pellicle inspired dendrimer. **Y. Xiao**, L. Jianshu

9:35 Intermission.

9:50 POLY **42.** Impact of particle modulus on vascular-targeted drug delivery *in vitro* and *in vivo*. **M. Fish**, C. Fromen, T.F. Scott, R. Adili, M. Holinstat, O. Eniola-Adefeso

10:20 POLY **43.** Kaolin-Polyurethane foam composites for multifunctional wound dressing applications. **J. Lundin**, G.C. Daniels, C.L. McGann, B. Streifel, S.L. Giles, J.H. Wynne

10:50 POLY **44.** Evolution of morphology in polyurethane biomaterials: Effect of time and storage on material properties. **E. Chen**, S. Eam, A. Padsalgikar

11:20 POLY **45.** Tuning surface properties of acrylate polymers to direct neurite growth. **B. Leigh**, K. Truong, R. Bartholomew, M.R. Hansen, A. Guymon

11:50 Concluding Remarks.

Section G

Moscone Center

Esplanade Ballroom 310

Contributions of IBM Almaden to Polymer Science

Cosponsored by PMSE

R. D. Miller, *Organizer*

D. Y. Yoon, *Organizer, Presiding*

R. Allen, *Presiding*

8:15 Introductory Remarks.

8:25 POLY **46.** Evolution of polymer science at IBM: From microelectronics to Watson Health. **J. Hedrick**

8:50 POLY **47.** High performance polymer and polymer/inorganic thermoelectric materials. **G. Hadziioannou**

9:15 POLY **48.** Surface-directed molecular assembly of organic semiconductors for organic electronics. **K. Cho**

9:40 POLY **49.** Multifunctional layers and memory devices based on ferroelectric polymers. **A.M. Jonas**

10:05 Intermission.

10:20 POLY **50.** Multiscale nanoparticle ordering by polymer crystallization. **S. Kumar**

10:45 POLY **51.** Controlled morphology and Its impact on digital memory behavior of well-defined functional polymers in nanoscale thin films. **M. Ree**

11:10 POLY **52.** Molecular relaxation studies of crystalline polymers, blends and copolymer networks. **D.S. Kalika**

11:35 POLY **53.** Big sticks and soft interactions (speaking of liquid crystals). **C. Viney**

Materials Informatics & Computational Modeling

Sponsored by CINF, Cosponsored by COMP and POLY

Frontiers in Nanoscience

Sponsored by SOCED, Cosponsored by POLY

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis, & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

New Horizons in Sustainable Materials

Renewable Polymers: Isolation, Structure & Properties

Sponsored by CELL, Cosponsored by POLY

SUNDAY AFTERNOON

Section A

Moscone Center

120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

F. Horkay, B. S. Lokitz, K. J. Wynne, *Presiding*

1:00 POLY **54.** Adaptive nanoparticles for regulation of endosomal signalling: Targeting pain at the source. **N. Veldhuis**, M. Whittaker, P. Ramirez-Garcia, Q. Mai, T. Lieu, N. Truong, J. Quinn, T. Davis, N.W. Bunnett

1:20 POLY **55.** Triggering cellular signalling processes with novel macromolecular hydrogen sulfide donors. F. Ercole, F. Mansfeld, M. Kavallaris, M. Whittaker, M. Halls, T. Davis, **J. Quinn**

1:40 POLY **56.** Toward a cure for facial acne without bacterial resistance buildup. **K.J. Wynne**, S. Nair, M. Beckwith, D. Ohman

2:00 POLY **57.** Synthesis and enviornmentally-responsive properties of poly(α-aminoesters): Applications for the delivery of messenger RNA. **T. Blake**, R.M. Waymouth

2:20 POLY **58.** Synthesis and biological evaluation of well-defined poly(propylene fumarate) oligomers and their use in 3D printed scaffolds. **Y. Luo**

3:00 POLY **59.** Molecularly imprinted polymers for high-density lipoprotein: Characterization and functionalization. **S. Chunta**, P. Lieberzeit

3:20 POLY **60.** Molecular interactions among cartilage proteoglycans. **F. Horkay**, P.J. Basser

3:40 POLY **61.** *Thermobifida cellulosilytica* cutinase as a powerful tool for the synthesis and functionalization of biobased polyesters. **A. Pellis**, E. Herrero Acero, V. Ferrario, L. Gardossi, G.M. Guebitz

4:00 POLY **62.** Modulating the hydrophobicity of cell penetrating peptide mimics for binding and intracellular delivery of protein cargo. **N.D. Posey**, L.M. Caffrey, L.M. Minter, G.N. Tew

4:20 POLY **63.** Novel self-assembled nanoparticle platform based on eight-arm-poly(ethylene glycol)-diosgenin prodrugs for co-delivery of anticancer drugs in cancer therapy. **C. Li**, **J. Lei**

4:40 POLY **64.** Recent developments in drug-loaded brush-arm star polymers. **M. Golder**, J.A. Johnson

Section B

Moscone Center

121

Carl S. Marvel Creative Polymer Chemistry Award in honor of Theresa M. Reineke

C. Lipscomb, T. J. White, *Organizers*

H. A. Klok, T. P. Lodge, *Presiding*

1:00 POLY **65.** Polymer-Based nanoparticle therapeutics. **M.E. Davis**

1:30 POLY **66.** Synthesis of rationally designed polymers for wound healing applications. **H.D. Maynard**

2:00 POLY **67.** Engineering cell surfaces with synthetic polymers. **H.A. Klok**

2:30 POLY **68.** Functional polycarbonates as oxidative- and pH-responsive materials. **M. Herrera-Alonso**

3:00 POLY **69.** Advances at the interface of catalyst design and polymer chemistry. **G.W. Coates**

3:30 POLY **70.** Biopolymeric conjugates in the design of hybrid biomaterials. **K.L. Kiick**

4:00 POLY **71.** Bio-inspired materials, synthesis and function. **C.J. Hawker**

4:30 POLY **72.** Designing tunable multifunctional macromolecules: From sustainable polymers to selective drug and gene delivery vehicles. **T.M. Reineke**

Section C

Moscone Center

122

Polymeric Materials for Performance & Sustainability

Functional Materials: Gels & Membranes

Cosponsored by MPPG‡

M. Meador, M. A. Meador, *Organizers*

S. E. Morgan, *Organizer, Presiding*

1:00 POLY **73.** Dynamics of solvent molecules in polyacrylate gels supported on a polymeric substrate. R. Islam, S. Mani, **R. Khare**

1:30 POLY **74.** Promising chemical stable membranes developed through combined effect of radical polymerization and non-solvent induced phase separation of acrylic functionalized polysulfone. **M.F. Mehmood**, S. Marco, P. Bosch, M. Giagnorio, A. Tiraferri

1:50 POLY **75.** Microfluidic spinning of polyethersulfone hollow fiber membranes. **K. Deng**, Z. Liu, F. Luo, R. Xie, X. Ju, W. Wang, L. Chu

2:10 POLY **76.** Efficient synthesis of functionalized shape-persistent ladder polymers for gas separation. **H.W. Lai**, Y. Teo, Y. Xia

2:30 Intermission.

2:45 POLY **77.** Super-Anisotropic swelling of hydrogels layered by domino-effects of cyanobacterial LC megamolecules. **M. Okajima**, T. Kaneko

3:05 POLY **78.** Siloxane-substituted polynorbornenes as advanced gas separation membranes. **B.K. Long**, K.R. Gmernicki, C. Maroon, M.A. Higgins

3:35 POLY **79.** CO_2-philic polymer membranes for high flux CO_2 separation. T. Hong, P. Cao, B. Li, S.M. Mahurin, D. Jiang, K. Vogiatzis, J.W. Mays, B.K. Long, A.P. Sokolov, **T. Saito**

3:55 POLY **80.** Mixed matrix materials containing Pd nanoparticles with superior membrane H_2/CO_2 separation properties. **H. Lin**, L. Zhu, D. Yin, S. Konda, M. Swihart

4:15 POLY **81.** pH-Sensitive linear amphiphilic block copolymers for transport and controlled release of molecular oxygen. **V.O. Rodionov**

Section D

Moscone Center

123

Separation of Macromolecules & Particulates

Cosponsored by ANYL, COLL and PMSE

Financially supported by PSS Polymer Standards Service GmbH, The Dow Chemical Company, Tosoh Bioscience LLC, Wyatt Technology

W. Gao, X. M. Liu, *Organizers*

S. V. Orski, Y. Wang, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 POLY **82.** Gel permeation chromatography of ultralarge polymers: Challenges and limitations. **D.M. Meunier**, Y. Li, W. Gao

1:45 POLY **83.** Detailed characterization of gelatins from different sources using aqueous gel permeation chromatography with on-line triple detection and multi-angle light scattering detection. **B. Crawshaw**, D. Herrick, W. Gao, X.M. Liu

2:15 POLY **84.** Characterization of biopolymer stability by size-exclusion chromatography and asymmetric flow field-flow fractionation. **Y. Li**, K. Kuppannan, M. Covington, D. Dodage, D.M. Meunier

2:45 Intermission.

3:00 POLY **85.** Composition and microstructure separations of polymers and nanoparticles using thermal field-flow fractionation. **K.R. Williams**, W.C. Smith, M.B. Pillion, K. Bierbaum, J. Oliver, C.R. Bria

3:40 POLY **86.** Separation and quantification of colloidal particles and polymers made by emulsion polymerization using asymmetrical flow field-flow fractionation with advanced detection: Challenges and progresses. **W. Gao**, S. Brownell, J. Bohling, P. Luo, A. Gong, K. Joshi, F. Zeng

4:10 POLY **87.** Correlation between structural properties and encapsulation efficiency in polymersomes. H. Gumz, S. Boye, D. Appelhans, **A. Lederer**

Section E

Moscone Center

124

Incorporating Polymer Science into the Classroom

High School & Community College

Cosponsored by CHED, MPPG‡ and PMSE

K. A. Cavicchi, *Organizer*

S. E. Morgan, *Organizer, Presiding*

K. Wingo, *Presiding*

1:00 POLY **88.** Developing polymer research lessons for the high school classroom – NSF RET at The University of Southern Mississippi. **K. Wingo**, S.E. Morgan

1:25 POLY **89.** Cross-linking physics and polymers: Making an impact in STEM education. **M. Boleware**, A. Sharma, J.S. Wiggins

1:50 POLY **90.** Synthesis and characterization of di(perylene bisimides) for use as an electron accepting material in polymer photovoltaic devices. **J. Brownlow**, T. Bullock, L. Moore, M. Norman, S.E. Morgan

2:15 POLY **91.** Innovation at the intersection of research and outreach. **K.A. Cavicchi**

2:40 Intermission.

2:55 POLY **92.** Augmenting primary and secondary education with polymer science and engineering. **R. Censonsky**, L. Foster, R.J. Hall, T. Ahn, H.L. van der Laan, T.F. Scott

3:20 POLY **93.** Polymers inspired by biomimetic bilayers. K.A. Cavicchi, **J. Oldham**

3:45 POLY **94.** Are mushrooms the new plastic? Harnessing student design thinking using ecovative materials. **M.C. Enright**, K. Anderson

4:10 POLY **95.** Exploring polymers in the high school classroom through medical sutures. **C. Knutson**, J.E. Wissinger, C. Javner, D.K. Schneiderman

Section F

Moscone Center

125

Polymer Applications & Characterization in the Biomedical Industry

X. M. Liu, J. Slager, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 POLY **96.** Graphene oxide-conjugated polymer hybrid materials for protein sensing. **C. Xing**

1:35 POLY **97.** Photo-curable betaine copolymer with high resistance to thrombus and biofilm formation. **Z. Zhang**, D. Wallach, J. Li, M. Taylor, A. Roussell, V. Wagner

2:05 POLY **98.** Self-fitting scaffolds based on PCL-PLLA semi-IPN Shape Memory Polymers (SMPs). **M. Grunlan**, L.L. Woodard, V.M. Page, K.T. Kmetz

2:35 Intermission.

2:50 POLY **99.** Effects of gel mass age on critical process parameters of soft gelatin capsule encapsulation. **M. Karamsetty**, R. Lau

3:20 POLY **100.** Photo-CuAAC applications in dental restorative materials. **B. El-Zaatari**, A. Shete, C.J. Kloxin

3:50 POLY **101.** All-organic conductive fabrics for continuous monitoring of Electrocardiogram (ECG) response. **G.A. Sotzing**

4:20 POLY **102.** Polymer materials in medical devices: Addressing issues through material testing and failure analysis. **S.J. Benight**

4:50 Concluding Remarks.

Section G

Moscone Center

Esplanade Ballroom 310

Contributions of IBM Almaden to Polymer Science

Cosponsored by PMSE

R. D. Miller, D. Y. Yoon, *Organizers*

K. R. Carter, J. Pyun, *Presiding*

1:00 POLY **103.** Polymers at interfaces. **T.P. Russell**

1:25 POLY **104.** Deposition, mechanics and phase behavior of polyelectrolyte complex films. **K.R. Shull**

1:50 POLY **105.** From industrial wastes to functional materials: Hybrid materials based on sulfur. **K. Char**

2:15 POLY **106.** Self-organization in materials science: From quantum dot LEDs to mechanical actuators. **R.W. Zentel**

2:40 POLY **107.** Synthesis and fabrication of functional polymer thin films. **K.R. Carter**

3:05 Intermission.

3:20 POLY **108.** From polymers to particles and back to polymers. **J. Pyun**, N.G. Pavlopoulos, N. Pinna, K. Char

3:45 POLY **109.** Multi-stimuli-responsive inks for 3D printing. **A. Nelson**

4:10 POLY **110.** Light-induced self-assembly of achiral molecules containing triphenylamine for supramolecular chirality and chiral polymers. **S.Y. Kim**

4:35 POLY **111.** From Almaden to Donostia: A trip from polymer brushes and self-crosslinking nanoparticles to poly(ionic liquid)s. **D. Mecerreyes**

5:00 POLY **112.** Research frontiers of the IBM Research Center as inspiration for the design of biological active materials. **E. Harth**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Materials Informatics & Computational Modeling

Sponsored by CINF, Cosponsored by COMP and POLY

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

New Horizons in Sustainable Materials

Nanocellulose Materials & 3D Structures

Sponsored by CELL, Cosponsored by POLY

MONDAY MORNING

Section A

Moscone Center

120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

T. M. Alam, P. Luo, *Presiding*

8:00 POLY **113.** Variable temperature ROMP: Achieving targeted molar mass and low dispersities from low ring-strain monomers. W.J. Neary, **J.G. Kennemur**

8:20 POLY **114.** Synthesis and characterization of aromatizing polyester. **W. Joo**, A. Lane, D. Liu, K. Matsuzawa, R.A. Mesch, W. Wang, B. Cassidy, A. Dick, S.T. Phillips, C.G. Willson

8:40 POLY **115.** Synthetic approach for reducing viscosity in commercially relevant polymer latexes. **P. Luo**, J. Bohling, K. Beshah

9:00 POLY **116.** Facile synthesis of robust, photopolymerizable liquid crystal elastomers. **N.P. Godman**, A.D. Auguste, T.J. White

9:20 POLY **117.** Versatile and general strategy to precision conjugated oligomers (PDI= 1.0). **J. Lawrence**, E. Goto, A. McGrath, D.S. Laitar, P. Clark, C.J. Hawker

9:40 POLY **118.** Effect of monomer solubility on the evolution of copolymer morphology during polymerization-induced self-assembly in aqueous solution. **A.A. Cockram**, T.J. Neal, M.J. Derry, O. Mykhaylyk, N.S. Williams, M.W. Murray, S.N. Emmett, S.P. Armes

10:00 POLY **119.** Impact of hydration and sulfonation on the nanoscale morphology of water in polyphenylene polymer membranes. **T.M. Alam**, E.G. Sorte, C. Fujimoto, L.J. Abbott, A.L. Frischknecht

10:20 POLY **120.** Innovations in the design and synthesis of charged polysulfones. **M. Green**, Y. Yang

10:40 POLY **121.** Thermoset in thermoplastic for shape memory polymer: Selective role for net point or switching segment under crosslink network. **S. Chirachanchai**

11:00 POLY **122.** Synthesis and characterization of waterborne, silane functional, branched polyerethanes for self-crosslinking coatings in textile applications. A. **Durmus**, D. Anil, E. Sevinis Ozbulut, Y.Z. Menceloglu, S. Unal

11:20 POLY **123.** Withdrawn.

11:40 POLY **124.** Linear multiblock copolymers with up to ten blocks and high molecular weights: A novel in-situ block copolymer formation approach. **E. Grune**, A. Mueller, H. Frey

Section B

Moscone Center

121

Next Generation Smart Materials

Cosponsored by MPPG‡

E. B. Berda, J. Foster, *Organizers*

Y. C. Simon, *Organizer, Presiding*

S. Camarero-Espinosa, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **125.** Multiresponsive polymers for drug delivery and sensors. **R. Hoogenboom**

8:35 POLY **126.** In Situ nanoparticlization of conjugated polymers. **T. Choi**

9:05 POLY **127.** Polymeric sulfothetins as solution responsive smart materials. **T. Emrick**

9:35 Intermission.

9:45 POLY **128.** Humidity- and electro-responsive actuation in anisotropically aligned protein films. **T. Zarkovic Grove**, N. Carter

10:15 POLY **129.** Smart biomimetic polymersomes. **S. Lecommandoux**

10:45 POLY **130.** Topological transformations via dynamic-covalent chemistry. H. Sun, C.P. Kabb, Y. Dai, M.R. Hill, **B.S. Sumerlin**

Section C

Moscone Center

122

Polymeric Materials for Performance & Sustainability

High Performance

Cosponsored by MPPG‡

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

J. Buchanan, *Presiding*

8:00 POLY **131.** Exceptional flame resistance and gas barrier with thick-growing clay-chitosan multilayer coatings. **J.C. Grunlan**, T. Guin

8:30 POLY **132.** Phosphorous-functionalized multi wall carbon nanotubes as flame retardants for polystyrene and poly (methyl methacrylate). **D.P. Durkin**, M.J. Gallagher, B.P. Frank, E.D. Knowlton, P.C. Trulove, D. Fox, H. Fairbrother

8:50 POLY **133.** Ultra-high thermostability in polybenzazoles from wholly-aromatic amino acid. **T. Kaneko**, M. Watanabe, M. Ali, M. Singh

9:10 POLY **134.** Hyperconnected network architectures as a new route to exceptional mechanical properties. **J. Burg**, R. Dauskardt

9:30 Intermission.

9:45 POLY **135.** Continuous manufacturing of twisted yarns from electrospun polymer fibers. W. Panatdasirisuk, **S. Yang**

10:05 POLY **136.** Catalyst optimization of covalent organic frameworks by frontier orbital engineering. **C.S. Diercks**, C.J. Chang, O.M. Yaghi, N. Kornienko, S. Lin

10:25 POLY **137.** Nanoscale toughening mechanism in MoS_2 dispersed epoxy composite system. J. Ryan, S. Webster, S. Roy, R. Wheeler, **D. Nepal**

10:45 POLY **138.** Moisture distribution in PEEK, PEKK, PBI, and their blends: A multinuclear solid-state NMR study. **J. Bluemel**, J.C. Pope

11:05 POLY **139.** Copolymerization of epoxides and lactones to ultrahigh molecular weight with an aluminum-chelate catalyst. **M. Chwatko**, N.A. Lynd

‡ *Cooperative Cosponsorship*

Section D

Moscone Center
123

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC

Financially supported by POLY Industrial Advisory Board

C. J. Ellison, T. E. Long, *Organizers*

H. Cheng, C. J. Landry-Coltrain, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **140.** Cooperative polymerization of α-helices induced by macromolecular architecture. **R. Baumgartner**, H. Fu, Z. Song, Y. Lin, J. Cheng

8:25 POLY **141.** Prebiotic depsipeptide formation from the ester-amide exchange reaction. **S. Yu**, R. Krishnamurthy, F.M. Fernandez, N.V. Hud, F.J. Schork, M. Grover

8:45 POLY **142.** Commodity plastic mimics from polyvinyl acetals derived from bioaromatic aldehydes and polyvinyl alcohol. **M. Rostagno**, S. Shen, I. Ghiviriga, S.A. Miller

9:05 POLY **143.** Sustainable antimicrobial biomaterials and biobased plastics from natural biomass. **M.S. Ganewatta**, C. Tang

9:25 POLY **144.** Efficient, regioselective path to water-soluble polysaccharide ionomers. **S. Liu**, K.J. Edgar

9:45 Intermission.

10:00 POLY **145.** Improving the biopharmaceutical properties of oligonucleotides by brush-polymer-assisted compaction. **X. Lu**, X. Cao, D. Wang, F. Jia, X. Tan, K. Zhang

10:20 POLY **146.** Complexation of linear DNA and polystyrene sulfonate with cationic copolymer micelles: Effect of polyanion flexibility. **Y. Jiang**, D. Sprouse, J. Lasser, T.M. Reineke, T.P. Lodge

10:40 POLY **147.** Photo-Responsive polymeric formulations to attenuate inflammation in cardiovascular tissues. **C.T. Greco**, T.H. Epps, M.O. Sullivan

11:00 POLY **148.** Functionalized star-like ε-caprolactone amphiphilic block copolymers for thermoresponsive micellar drug delivery systems. **K.E. Washington**, R.N. Kularatne, Y. Ren, M.C. Biewer, M.C. Stefan

Section E

Moscone Center
124

Undergraduate Research in Polymer Science

J. Lott, S. E. Morgan, S. I. Nazarenko, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **149.** Multi-scale assembly of polythiophene-surfactant supramolecular complexes. **D. Bilger**, A. Sarkar, C.D. Danesh, M. Gopinadhan, G. Braggin, J. Figueroa, T. Pham, D. Chun, Y. Rao, C.O. Osuji, M. Stefik, S. Zhang

8:25 POLY **150.** Polyureas for dielectric applications developed through a rational co-design approach. **S.K. Scheirey**, G.M. Treich, S. Nasreen, Z. Li, A. Mannodi-Kanakkithodi, Y. Cao, R. Ramprasad, G.A. Sotzing

8:45 POLY **151.** Incorporation of Diels-Alder chemistry into polymer matrices via an inimer approach. **T. Colt**, K. Barcus, E. Crenshaw, R. Rhoads, **P.J. Costanzo**

9:05 POLY **152.** Stimuli responsive β-cyano-oligo(phenylene vinylene) methylcellulose hydrogels. **L. Forte**, B. Davis, J. Lott

9:25 Intermission.

9:45 POLY **153.** Thio-bromo click approach for developing new, ROMP-based flame-resistant materials. **J. Grubb**, C.E. Hobbs

10:05 POLY **154.** Utilization of a cysteine core for the preparation of novel mikto-arm star polymer. **C. Sarantes**, K. Eckhart, C. DeHoe, L. Souza, A. Ventura, A.J. Varni, **P.J. Costanzo**

10:25 POLY **155.** Alkynols as a source of flame retardants. **A. Gudbrandson**, B. Howell

Section F

Moscone Center
Esplanade Ballroom 310

50th Anniversary Celebration of Macromolecules

Cosponsored by MPPG‡ and PMSE

T. P. Lodge, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 POLY **156.** Self-assembled supramolecular nanosystems for smart diagnosis and targeted therapy of intractable diseases. **K. Kataoka**

8:40 POLY **157.** Electrostatic assembly of nanoparticle systems for controlled and tissue targeted release. **P.T. Hammond**

9:10 POLY **158.** Toughening soft materials with sacrificial bonds. **J.P. Gong**

9:40 Intermission.

10:00 POLY **159.** Principles of vitrimer chemistry and physics. **L. Leibler**

10:30 POLY **160.** How advances in polymer synthesis have enabled advances in polymer physics. **K.I. Winey**

11:00 POLY **161.** Entropic barrier theory of dynamics of macromolecules. **M. Muthukumar**

Section G

Moscone Center
125

Contributions of IBM Almaden to Polymer Science

Cosponsored by PMSE

D. Y. Yoon, *Organizer*

R. D. Miller, *Organizer, Presiding*

T. P. Russell, *Presiding*

8:00 POLY **162.** Story of single-molecule detection and spectroscopy and the surprises leading to super-resolution microscopy and beyond. **W.E. Moerner**

8:30 POLY **163.** Learning from nature to create novel nanomaterials. **R.K. OReilly**

8:55 POLY **164.** Supramolecular biomaterials: From fundamentals to advanced healthcare solutions. **E.A. Appel**

9:20 POLY **165.** Applications of functionalized biodegradable polymers in tissue engineering and regenerative medicine. **K. Fukushima**, Y. Inoue, Y. Haga, M. Oji, S. Takaoka, C. Sato, H. Tsuchiya, M. Tanaka

9:45 POLY **166.** Degadable elastomeric biomaterials through stereochemically-controlled synthesis. **A.P. Dove**

10:10 Intermission.

10:25 POLY **167.** Forty years of spectroscopic studies of polymers at the leading edge from FT-Raman to AFM-IR spectroscopy: Evolution, revolution or back to the future. **J.F. Rabolt**

10:50 POLY **168.** Development of multi-functional surfaces with controllable wettability. M.A. Frysali, G. Kenanakis, G. Kaklamani, L. Papoutsakis, **S.H. Anastasiadis**

11:15 POLY **169.** Developments in polymer adhesion and fracture at IBM Almaden Reseach Laboratory. **H.R. Brown**

11:40 POLY **170.** Effects of molecular topology and interface on conformations and dynamics of polymer melts from atomistic molecular dynamics simulations. **D.Y. Yoon**

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY AFTERNOON

Section A

Moscone Center
120

Industrial Innovations in Polymer Chemistry

Cosponsored by MPPG‡ and PMSE

T. W. Baughman, *Organizer*

J. M. Messman, *Organizer, Presiding*

1:00 POLY **171.** Development of silicon-containing polymers for modern micro- and nano-electronics. **Q. Lin**

1:30 POLY **172.** Advances in Asymmetric Flow Field Flow Fractionation (AF4) combined with MALS in the characterization of polymers in solution. **J.A. Ahlgren**

2:00 POLY **173.** Cognitive macromolecular therapeutics. **J. Hedrick**

2:30 Intermission.

2:45 POLY **174.** Development of sustainable alternatives for the next generation of chemicals and materials: Continued progress in development of renewably-sourced materials from DuPont. **H.E. Bryndza**

3:15 POLY **175.** Future fabricated with light: Photolithography in 2D leading to CLIP in 3D. **J.M. DeSimone**

3:45 POLY **176.** Digital manufacturing at the NNSA's National Security Campus. **D.E. Bowen**

Section B

Moscone Center
121

Next Generation Smart Materials

Cosponsored by MPPG‡

J. Foster, Y. C. Simon, *Organizers*

E. B. Berda, *Organizer, Presiding*

T. Zarkovic Grove, *Presiding*

1:00 Introductory Remarks.

1:05 POLY **177.** Stimuli-responsive metal organic framework nanoparticles. **A.J. Morris**, C.C. Epley

1:35 POLY **178.** Atypical responses from polymeric nanoassemblies. **S. Thayumanavan**

2:05 POLY **179.** Molecular design strategies for smart materials based on new dynamic bonding motifs in polymers. **B. Helms**

2:35 Intermission.

2:45 POLY **180.** Engineering multi-responsive complex coacervate core micelles for biomedical and materials science applications. **I. Voets**

3:15 POLY **181.** Processing effects on mechanically adaptive response of cellulose nanocrystal composites. **M. Bortner**, J. Foster, J. Fallon, B. Kolb, C. Herwig

3:45 POLY **182.** Self-Assembly and responsiveness of polypeptide-based star and triblock copolymers. C. Machado, I. Smith, B. Barnes, **D.A. Savin**

4:15 POLY **183.** Nanoparticle assembly of surface-modified proteins. M. Fach, L. Radi, **P.R. Wich**

Section C

Moscone Center
122

Polymeric Materials for Performance & Sustainability

Biodegradable & Recyclable Polymers

Cosponsored by MPPG‡

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

B. Schmatz, *Presiding*

1:00 POLY **184.** Recyclable crosslinked polymer networks via one-step controlled radical polymerization: Full property recovery after multiple melt-reprocessing steps of models for tire rubber and other polymer networks. **J.M. Torkelson**, K. Jin, L. Li

1:30 POLY **185.** Compounding of thermoplastic polysaccharides and biodegradable polyesters. **B. Zhou**, J.H. Wang, Q. Jia

1:50 POLY **186.** Biodegradable polyesters/cellulose esters blends: Thermal and rheological properties important for thermoplastic processing. **Y. Bai**, J.H. Wang, J. Kuang, B. Zhou

2:10 POLY **187.** Renewable silicon-containing cross-linked polymers and tuning their properties. **Y. Nishimura**, J. Chung, Z. Guan

2:30 Intermission.

2:45 POLY **188.** Biodegradable compolymers based on poly(ε-caprolactone): From packaging to wastewater treatment applications. **M.K. Hassan**, H. Qayouh, E. Jacob, K. Zadeh, S.A. Al-Muhtaseb, M.A. Al-Maadeed, M. Lahcini

3:05 POLY **189.** Stress relaxation and reprocessability of cross-linked polyhydroxyurethanes. **D.J. Fortman**, J.P. Brutman, M.A. Hillmyer, W.R. Dichtel

3:25 POLY **190.** Polycarbonate vitrimers from bis(cyclic carbonates) and polyols. **R.L. Snyder**, D.J. Fortman, W.R. Dichtel

3:45 POLY **191.** Renewable aliphatic-aromatic copolyesters based on phloretic acid. **M.J. Miri**, M.E. Bloom, J.F. Vicentin, J.M. Marsico, T.S. Geraci, D.S. Honeycutt

4:05 POLY **192.** Structure-property relationships in modified highly functional bio-based thermosets. **A.Z. Yu**, J.M. Sahouani, D.C. Webster

Section D

Moscone Center

123

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC

Financially supported by POLY Industrial Advisory Board

H. Cheng, C. J. Landry-Coltrain, *Organizers*

C. J. Ellison, T. E. Long, *Organizers*, *Presiding*

1:00 Recogntion of Poster Presenters.

1:15 POLY **193.** Mechanically stiff 3D printed biomimetic hydrogel for chondrogenesis and cartilage tissue production. **E. Aisenbrey**, S.J. Bryant

1:35 POLY **194.** Exciton migration in conjugated polymers at the amphiphilic interfaces. **B. Koo**, T.M. Swager

1:55 POLY **195.** Molecular engineering of polymers to realize high thermal conductivity in amorphous systems. **A. Shanker**, G. Kim, C. Li, K. Pipe, J. Kim

2:15 POLY **196.** Directed structure manipulation of conjugated polymers with external fields. **Y. Xi**, L.D. Pozzo

2:35 Intermission.

2:50 POLY **197.** Direct, single-step alignment of semiconducting polymer thin films and factors influencing their deposition via solution shearing. **L. Shaw**, P. Hayoz, H. Yan, Y. Diao, J. Reinspach, J.W. To, M. Toney, T. Weitz, Z. Bao

3:10 POLY **198.** Direct formation of large area two-dimensional nanosheets from fluorescent semi-conducting homopolymer with new orthorhombic crystalline orientation. **S. Yang**, I. Choi, S. Shin, T. Choi

3:30 POLY **199.** Directed self-assembly of 5 nm block copolymer lamellae enabled by nanoimprint lithography. **A. Lane**, X. Yang, M.J. Maher, G. Blachut, Y. Asano, Y. Someya, S. Sirard, A. Mallavarapu, C.J. Ellison, C.G. Willson

3:50 POLY **200.** Quantitative predictions of shape memory effects in polymers. **C.C. Hornat**, Y. Yang, M.W. Urban

Technical program information known at press time.
The official technical program for the 253rd ACS National Meeting is available at:
www.acs.org/SanFran2017

Section E

Moscone Center

124

Undergraduate Research in Polymer Science

J. Lott, S. E. Morgan, S. I. Nazarenko, *Organizers*, *Presiding*

1:00 POLY **201.** Semi-flexible string conformational analysis towards an experimental hydrophobic-folding model system. **R. Kiessling**, C. Barraugh, B. Sanii

1:20 POLY **202.** pKa determination of a his residue in a self-assembling peptide using Raman spectroscopy. **B. Pogostin**, C.H. Londergan, K.S. Akerfeldt

1:40 POLY **203.** Aligned spherulites of conjugated polymers induced by carbon nanotubes. **K.J. Reynolds**, S. Zhang

2:00 Intermission.

2:20 POLY **204.** Thermally responsive materials with dynamic topology based upon Diels-Alder chemistry. **C. Gregory**, E. Wilborn, **P.J. Costanzo**

2:40 POLY **205.** Thermal and flammability properties of epoxy resin containing flame retardants derived from castor oil. **E. Ostrander**

3:00 POLY **206.** Modular liquid crystal elastomer synthesis: Acid catalyzed oxa-Michael addition. **C. Earl**, Z. Kurji, J.A. Kornfield

3:20 Intermission.

3:30 Panel Discussion.

Section F

Moscone Center

Esplanade Ballroom 310

50th Anniversary Celebration of Macromolecules

Cosponsored by MPPG‡ and PMSE

T. P. Lodge, *Organizer, Presiding*

1:00 POLY **207.** Syntheses, structures and functions of AIE polymers. **B. Tang**

1:30 POLY **208.** Polymer chemistry of graphenes and graphene nanoribbons. **K. Muellen**

2:00 POLY **209.** Digital polymers: A new class of man-made macromolecules. **J. Lutz**

2:30 Intermission.

2:50 POLY **210.** Historical evolution of degradable polymers in the Wooley laboratory: From poly(silyl ester)s to natural product-based polycarbonates. **K.L. Wooley**

3:20 POLY **211.** Reversible deactivation radical polymerization after nearly 50 years. **K. Matyjaszewski**

3:50 POLY **212.** 50 Years of macromolecules: A perspective. **T.P. Lodge**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

C. Lipscomb, *Organizer*

8:00 - 10:00

245, 329-330, 342, 345-348, 351, 353, 355, 357-358, 364-365, 367, 371, 373-378, 383, 385, 388, 390-391, 393, 395, 397-398, 406-407, 421, 424, 428, 430-431, 433-435, 441-442, 453-455, 459, 461-464, 467, 469, 474-475, 477-478. See subsequent listings.

Innovating Materials for the Next Generation: Bringing Practical Applications into the Chemistry Classroom

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

TUESDAY MORNING

Section A

Moscone Center

120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

D. S. Dissanayake, D. A. Waldow, *Presiding*

8:00 POLY **213.** Diffusion-Ordered NMR Spectroscopy (DOSY) of conjugated polymers. **L.M. Kozycz**, C.J. Hawker, M.L. Chabinyc

8:20 POLY **214.** Fiber-coupled NMR: A simple and versatile approach to study controlled photopolymerizations in real time. **N. Dolinski**, Z.A. Page, F. Eisenreich, S. Hecht PhD, J. Read De Alaniz, C.J. Hawker

8:40 POLY **215.** PFPE-based polymeric ^{19}F MRI agents: A new class of contrast agents with outstanding sensitivity. **C. Zhang**, H. Peng, S. Puttick, D. Searles, A. Whittaker

9:00 POLY **216.** Decoupling of segmental motion and ionic conductivity in oligomeric ethylene oxide functionalized dicarboxide oxanorbornene polymers. **D.A. Waldow**, A.P. Sokolov, Y. Wang

9:20 POLY **217.** Light scattering without refractive index increment. A new approach to calibrate SEC-light scattering setups. **W. Radke**, J. Preis, S. Lavric

9:40 POLY **218.** Polyimide-Tin(poly) ester hybrid films as dielectric materials. **S. Nasreen**, G.M. Treich, M.L. Baczkowski, M. Tefferi, S.K. Scheirey, Y. Cao, G.A. Sotzing

10:00 POLY **219.** Chemically degradable polymers for applications in nano and biotechnology. **I. Kolesnichenko**, C. Ginestra, M. Chwatko, J. Reuther, N. Lynd, E.V. Anslyn

10:20 POLY **220.** Particles formed from poly(butyl methacrylate)-co poly(acrylic acid). **S. Rimmer**, S.L. Canning, M. Geoghegan

10:40 POLY **221.** Triethylene glycol monomethyl ether substituted polythiophenes for organic electronic applications. **D.S. Dissanayake**, S.S. Gunathilake, J. Du, T.M. Pathiranage, E. Sheina, E. Gomez, M.C. Stefan, M.C. Biewer

11:00 POLY **222.** Withdrawn.

11:20 POLY **223.** Synthesis and characterization of highly branched, functional poly(arylene ether sulfone)s. **E. Sevinis Ozbulut**, A. Ozture, I. Sacligil, T. Ormanci Acar, D. Imer, I. Koyuncu, Y.Z. Menceloglu, S. Unal

11:40 POLY **224.** Can the overall molecular architectures of synthetic polymers be characterized ? R. Gurarslan, **A.E. Tonelli**

Section B

Moscone Center

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Next Generation Smart Materials

Cosponsored by MPPG‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

M. Bortner, A. Ostrowski, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **225.** Glucose-tactic asymmetric polymersomes. **G. Battaglia**

8:35 POLY **226.** Design strategy for efficient intramolecular singlet fission in oligoacenes. **E. Kumarasamy**, L. Campos

9:05 POLY **227.** Electrspun phase separating block-copolymer fibers for biological applications. **S. Camarero-Espinosa**, J. Cooper-White

9:35 Intermission.

9:45 POLY **228.** Functional molecular vibrations for stimuli responsive polymers. **J. Lott**

10:15 POLY **229.** Bio-Inspired porous amphiphobic materials through surface step-growth polymerization. S. Oyola-Reynoso, J. Chen, B. Chang, I. Tevis, **M. Thuo**

10:45 POLY **230.** Controlling mechanical properties of polymeric materials using photo-active metal coordination interactions. **A. Ostrowski**

11:15 POLY **231.** Examining the mechanical reactivity of substituted cylobutene mechanophores. **C.L. Brown**, T.B. Kouznetsova, B. Bowser, S. Craig

‡ *Cooperative Cosponsorship*

Section C

Moscone Center
122

Polymeric Materials for Performance & Sustainability

Functional Materials for Energy & Electronics

Cosponsored by MPPG‡

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

B. Long, *Presiding*

8:00 POLY **232.** Light on an upward trajectory: Sensitized light upconversion in polymers. **Y.C. Simon**

8:30 POLY **233.** Conjugated polyelectrolytes as light harvesting antenna. **C. Segura**, A. Ayzner

8:50 POLY **234.** Chlorination: A facile method for high-performance polymer solar cells. **F. He**

9:10 POLY **235.** Effect of solvent vapor annealing on crystallinity and hole mobility in P3HT:PCBM polymer photovoltaics. **L. Moore**, M. Bhattacharya, Q. Wu, S. Youm, E.E. Nesterov, S.E. Morgan

9:30 POLY **236.** Enhancing charge transport in redox active polymers through molecular design. **K. Hernandez-Burgos**, M. Burgess, E. Chenard, N. Gavvalapalli, R. Assary, J. Moore, J. Rodriguez Lopez

9:50 Intermission.

10:05 POLY **237.** Multi-grafting lithium polyacrylate as high-performance polymer binder for lithium-ion battery. **P. Cao**, M. Abdelmalak, E. Stacy, B. Li, T. Hong, J. Nanda, A.P. Sokolov, T. Saito

10:25 POLY **238.** Drifting proton transport by nanophase separation induced intrinsic electric field in polymer electrolyte material under anhydrous state. **Y. Hu**, L. Yan, B. Yue

10:45 POLY **239.** Photophysical changes driven by complexation of oppositely charged conjugated polyelectrolytes. **W.R. Hollingsworth**, C. Segura, J. Balderrama, N. Lopez, P. Schleissner, A. Ayzner

11:05 POLY **240.** Application of polypyrrole-based selective electrodes in electrochemical impedance spectroscopy to determine nitrate concentration. **M.C. So**, M. Hajimorad, H. Mustafa, S. Alhloul

Section D

Moscone Center
123

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC

Financially supported by POLY Industrial Advisory Board

C. J. Landry-Coltrain, T. E. Long, *Organizers*

H. Cheng, C. J. Ellison, *Organizers*, *Presiding*

8:00 POLY **241.** Consequences of low-χ design in block copolymer self-assembly. **A. Chang**, R.H. Grubbs

8:20 POLY **242.** Development and applications of living alternating ring-opening metathesis polymerization of cyclopropenes. **B.R. Elling**, Y. Xia, J. Su

8:40 POLY **243.** Graft-through synthesis and assembly of Janus bottlebrush polymers from A-branch-B diblock macromonomers. **K. Kawamoto**, M. Zhong, K.R. Gadelrab, L. Cheng, C.A. Ross, A. Alexander-Katz, J.A. Johnson

9:00 POLY **244.** Strong aliphatic polyester thermoplastic elastomers. **A. Watts**, M.A. Hillmyer

9:20 POLY **245.** Synthesis and characterization of bottlebrush polymers: The importance of the Anchor Group. **S. Radzinski**, J. Foster, R. Chapleski Jr, D. Troya, J. Matson

9:40 Intermission.

9:55 POLY **246.** Thiol-ene/yne photopolymerization – Simple reactions to yield complex materials. **D.V. Amato**, D.L. Patton

10:15 POLY **247.** Chain-growth CuAAC polymerization: A versatile strategy to produce hyperbranched polymers with well-defined structures in one-pot. **X. Cao**, Y. Shi, W. Gan, H. Naguib, X. Wang, R. Graff, H. Gao

10:35 POLY **248.** Water-Soluble ion-containing poly(ether ester)s for extrusion 3D printing. **A. Pekkanen**, C. Zawaski, C.B. Williams, T.E. Long

10:55 POLY **249.** Recyclable cross-linked polymer networks via one-step controlled radical polymerization. **K. Jin**, L. Li, J.M. Torkelson

Section E

Moscone Center
124

Structure to Function in Supramolecular Polymers & Materials

R. Kieltyka, J. B. Matson, *Organizers*

P. Besenius, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 POLY **250.** Living crystallization-driven, seeded growth approaches to functional supramolecular materials. **I. Manners**

8:30 POLY **251.** Living supramolecular polymerization of perylene bisimide J-aggregates. **W.J. Wagner**, **V. Stepanenko**, **F. Wuerthner**

8:50 POLY **252.** Probing hydrogen bond-aromaticity coupling in squaramide-based supramolecular polymers. **R. Kieltyka**

9:15 POLY **253.** Supramolecular polymers in aqeous media: From mechanisms to materials. **B. Rybtchinski**

9:40 Intermission.

9:55 POLY **254.** Zerovalent metallosupramolecular polymers for the in situ nucleation of platinum nanoparticles. **L. Montero de Espinosa**, L. Olaechea, C. Weder

10:20 POLY **255.** Network structure-property relationships in polymer metal-organic-cage gels. **A.V. Zhukhovitskiy**, J. Zhao, M. Zhong, E.G. Keeler, E. Alt, P. Teichen, R.G. Griffin, M.J. Hore, A. Willard, J.A. Johnson

10:40 POLY **256.** Metallo-Supramolecular crosslinked elastomers. **R.H. Lambeth**, A.M. Savage, F.L. Beyer

11:00 POLY **257.** Porous functional nanostructures mediated by directed supramolecular interactions. **F. Beuerle**

11:25 POLY **258.** Dynamic, multi-stimuli-responsive polymers based on metal-stabilized, dynamic covalent imine bonds. F. García, J. Pelss, H. Zuilhof, **M. Smulders**

Section F

Moscone Center
125

Polymer Chemistry (RSC) Lectureship

Cosponsored by MPPG‡

Financially supported by Royal Society of Chemistry, Tosoh

J. A. Johnson, E. Pentzer, W. You, *Organizers*

J. Kalow, E. Kumarasamy, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **259.** Hybrid nanomaterials. **R.K. OReilly**

8:35 POLY **260.** Design and synthesis of polymers for next generation energy storage technologies. **B.P. Fors**

8:55 POLY **261.** Mechanochemical generation of conjugated polymers from non-conjugated polymers. Z. Chen, J.A. Mercer, N.Z. Burns, **Y. Xia**

9:15 POLY **262.** Polymers for thermal and mechanochemical release of nitroxyl (HNO) and other small molecule payloads. D. Church, S. Nourian, C. Lee, M. Ryskamp, A. Vander Meer, N.A. Yakelis, J.P. Toscano, **A.J. Boydston**

9:35 Intermission.

9:55 POLY **263.** Functionally-versatile polypeptide materials. J. Fan, X. He, R. Letteri, T. Nguyen, J. Zou, **K.L. Wooley**

10:25 POLY **264.** Bioinspired sequence-defined oligomers and their biological applications. **C.A. Alabi**

10:40 POLY **265.** Designer molecules toward advanced polymerizations: Control of sequence and topology for vinyl polymers. **M. Ouchi**

11:00 POLY **266.** α,ω-Difunctional polyethylene telechelics through functional group tolerant catalysis. **S. Mecking**

Polymers under Deformation

Structure & Morphology Changes during Deformation of Polyolefins & Polymer Composites

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

TUESDAY AFTERNOON

Section A

Moscone Center
120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

A. Prasher, G. M. Treich, *Presiding*

1:00 POLY **267.** Organocatalyzed synthesis of polyurethanes. H. **Sardon**, A. Bossion, A. Yuen

1:20 POLY **268.** Aqueous copper(II) photoinduced polymerization of acrylates: Low copper concentration and the importance of sodium halide salts. **G.R. Jones**, R. Whitfield, A. Anastasaki, D.M. Haddleton

1:40 POLY **269.** Synthesis, characterization, and analysis of a novel polythiourea for dielectric applications aided by molecular dynamics and density functional theory. **G.M. Treich**, M. Misra, S. Nasreen, M. Tefferi, A. Mannodi-Kanakkithodi, R. Ramprasad, Y. Cao, G.A. Sotzing

2:00 POLY **270.** Controlled ring-opening polymerization of *O*-carboxyanhydrides using organometallic catalysts. **R. Tong**, J. Cheng

2:20 POLY **271.** Synthesis of vinylic macromolecular rotaxane cross-linkers endowing network polymers with toughness. **J. Sawada**, D. Aoki, T. Takata

2:40 POLY **272.** Topology transformation from linear polymer to cyclic Polymer: Effective synthesis of cyclic polymer utilizing [c2]daisy chain dimer. **D. Aoki**, T. Takata

3:00 POLY **273.** Wrinkling polymer brush surfaces via postpolymerization modification. **C. Reese**, W. Guo, L. Xiong, C.M. Stafford, B.S. Lokitz, O. Ovchinnikovo, A. Ievlev, D.L. Patton

3:20 POLY **274.** Methanol-mediated living cationic polymerization of 4-methoxystyrene via oxonium intermediate. **A. Prasher**, S.R. Liffland, D.A. Nicewicz, W. You

3:40 POLY **275.** Withdrawn.

4:00 POLY **276.** Synthesis and characterization of diamondoid substituted block copolymers. **C. Hill**, M.F. Roll

4:20 POLY **277.** Design and synthesis of new initiators for the ring opening polymerization of epoxides inspired by the Vandenberg catalyst. **N.A. Lynd**

4:40 POLY **278.** Isospecific, chain shuttling polymerization of propylene oxide using a bimetallic chromium catalyst: A new route to semicrystalline polyols. **M. Childers**, L.S. Morris, G.W. Coates

Section B

Moscone Center
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Next Generation Smart Materials

Cosponsored by MPPG‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

J. Lott, A. Ostrowski, *Presiding*

1:00 Introductory Remarks.

1:05 POLY **279.** Chromonic liquid crystal hydrogels. **R. Kularatne**, T.H. Ware

1:25 POLY **280.** Self-Assembly and phase behavior in mixed polymer brushes. **C.K. Simocko**, A.L. Frischknecht, D. Huber

1:45 POLY **281.** Materials for drug capture: Filtering off-target chemotherapy agents from the bloodstream. **M.D. Schulz**, C. Blumenfeld, S. Hetts, R.H. Grubbs

2:05 POLY **282.** Multifunctional cellulose ether derivatives for high performance amorphous solid dispersions prepared by olefin cross-metathesis and thiol-michael addition. **Y. Dong**, L.I. Mosquera-Giraldo, L. Taylor, K.J. Edgar

2:25 POLY **283.** Synthesis and characterization of organic ion-pairs as dynamic bonds for stimuli-responsive polymers. **G. Deng**, K.A. Cavicchi

2:45 Intermission.

2:55 POLY **284.** Optical devices constructed from smart microgels for sensing. **Q.M. Zhang**, S. Mugo, M. Serpe

3:15 POLY **285.** Antifouling aminoplast coatings and their layer-by-layer deposition technique. **M. Fevre**, X. Ding, R. Wojtecki, Y. Yang, J. Hedrick

3:35 POLY **286.** Polymeric sensors for 6-D super-resolution microscopy: Advanced fluorogenic materials for measuring redox reactions at surfaces and in solution. **J. Cole**, A. Hanlon, E.B. Berda

3:55 POLY **287.** Functionalized poly(propylene fumarate) for 3D printed bone growth scaffolds. **J. Wilson**, A. Kleinfehn, S. Petersen, Y. Chen, M. Becker

4:15 POLY **288.** Vesicle-to-worm transition provides a new high-temperature oil thickening mechanism. **M.J. Derry**, O. Mykhaylyk, S.P. Armes

Section C

Moscone Center

122

Polymers & Biomimicry

A. N. Dhinojwala, T. Williams, *Organizers*, *Presiding*

1:00 POLY **289.** Tough antibiotic-eluting double network hydrogels. **R. Stewart**, D. Lane

1:30 POLY **290.** Polysulfonates with complex architectures as heparin mimics. B. **Caroline**, R. Peltier, H. Kim, A. Mastrangelo, S. Perrier

1:50 POLY **291.** Nature-inspired hydrogels that change shape in response to external stimuli or to specific biomolecules. **S.R. Raghavan**

2:10 POLY **292.** Synthesis of a super-agonist heparin-mimicking block copolymer-FGF2 conjugate. **S. Paluck**, T.H. Nguyen, J.P. Lee, H.D. Maynard

2:30 POLY **293.** Triazole polypeptides: Regulation of polypeptide conformation through side-chain hydrogen bonding patterns. **Z. Song**, R.A. Mansbach, R. Baumgartner, A. Ferguson, J. Cheng

2:50 Intermission.

3:00 POLY **294.** Bio-inspired metal-coordination dynamics: An easy way to engineer gel viscoelastic mechanics. **N. Holten-Andersen**

3:30 POLY **295.** Crosslinking acrylate-containing polymers by downstream piezoelectric reduction. **E. Sanders**, H. Mohapatra, A.P. Esser-Kahn

3:50 POLY **296.** Superhydrophobic coatings from Treated diatomaceous earth. **F.D. Blum**, B.R. Sedai, H. Perera, A. Paul, B.K. Khatiwada, H. Mortazavian

4:10 POLY **297.** Protein-mimetics materials based on styrene-maleic anhydride copolymers. **A.A. Smith**, S.M. Darnall, A. Hall, **M. Puga**, T. Xu

Section D

Moscone Center

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Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC

Financially supported by POLY Industrial Advisory Board

H. Cheng, C. J. Ellison, *Organizers*

C. J. Landry-Coltrain, T. E. Long, *Organizers*, *Presiding*

1:00 POLY **298.** Accessing poly(olefin)-block-poly(thiophene) copolymers via one-pot living polymerizations. **A. Leone**, K. Souther, A.J. McNeil

1:20 POLY **299.** Distinct thermophysical and interfacial properties associated with low molecular weight cyclic polystyrene in bulk and confined states: T_g, fragility, and thin film stability. **L. Zhang**, R. Elupula, S.M. Grayson, J.M. Torkelson

1:40 POLY **300.** Unzipping polyester as a new photoresist material. **W. Joo**, A. Lane, D. Liu, K. Matsuzawa, R.A. Mesch, W. Wang, B. Cassidy, A. Dick, S.T. Phillips, C.G. Willson

2:00 POLY **301.** Organocatalyzed atom transfer radical polymerization via photoredox catalysis. **R.M. Pearson**, G. Miyake

2:20 Intermission.

2:35 POLY **302.** Simple, generalizable method towards highly aligned functional polymeric films. **Z. Qiang**, K.A. Cavicchi, B.D. Vogt

2:55 POLY **303.** High oxygen gas barrier multilayer thin films through pH and ionic strength manipulation of montmorillonite clay. **Y. Song**, D. Hagen, J.C. Grunlan

3:15 POLY **304.** Controlling and manipulating crease formation in polymer brush platforms. **K. Brooks**, M.J. Razavi, X. Wang, J.J. Locklin

3:35 POLY **305.** Tuning CO_2-philicity in highly permeable polymeric membranes for gas separation. **T. Hong**, H. Feng, S. Lai, S.M. Mahurin, D. Jiang, B.K. Long, J.W. Mays, A.P. Sokolov, T. Saito

Section E

Moscone Center

124

Structure to Function in Supramolecular Polymers & Materials

P. Besenius, *Organizer*

R. Kieltyka, J. B. Matson, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 POLY **306.** Self-Assembly of exfoliated monolayer crystals as photoswitchable soft matter. **R.H. Zha**, J.A. Berrocal, G. Vantomme, R. Gosens, B. de Waal, E.W. Meijer

1:30 POLY **307.** N-annulated perylenes. Outstanding scaffolds to build up functional supramolecular polymers. **L. Sánchez**, J. Buendía, E. Greciano, J. Valera, Y. Dorca, R. Gómez

1:55 POLY **308.** Controlling the assembly of multicomponent supramolecular gelator systems. E. Draper, C. Colquhoun, E. Cross, **D. Adams**

2:20 POLY **309.** Supramolecular control over thermoresponsive polymers. **R. Hoogenboom**

2:45 POLY **310.** Control of functional materials and supramolecular network dynamics at both the molecular and colloidal length scales. **O.A. Scherman**

3:10 Intermission.

3:25 POLY **311.** Functional materials from self-assembled *bis*-urea macrocycles. **L.S. Shimizu**, S.R. Salpage, B. Som, A.J. Sindt

3:50 POLY **312.** Impact of solvency and secondary structure on the conformation of single chain polymeric nanoparticles. G. ter Huurne, L. de Windt, A. Palmans, E.W. Meijer, **I. Voets**

4:15 POLY **313.** Single-chain nanoparticles with sequenced defined segments via multicomponent reactions. **E.B. Berda**, J. Cole

4:40 POLY **314.** Controlled self-assembly of peptidic Au(I)-metalloamphiphiles into 1D nanorods in water. **B. Kemper**, P. Besenius

5:00 POLY **315.** Photo- and magnetoresponsive self-assembly of nanoparticles. **B. Ravoo**

Section F

Moscone Center

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Polymer Chemistry (RSC) Lectureship

Cosponsored by MPPG‡

Financially supported by Royal Society of Chemistry, Tosoh

J. A. Johnson, E. Pentzer, W. You, *Organizers*

A. Anastaski, W. Gutekunst, *Presiding*

1:00 Introductory Remarks.

1:05 POLY **316.** Poly(2-oxazoline)s as functional biomaterials. **R. Hoogenboom**

1:35 POLY **317.** Training the old dog new tricks: The applications of the Biginelli reaction in polymer chemistry. **L. Tao**

1:55 POLY **318.** Biomass-derived polymers incorporating hydroxycinnamates. **A.M. Kasko**

2:10 POLY **319.** Polymeric materials for delivery of hydrogen sulfide (H_2S), a biologically relevant signaling gas. **J.B. Matson**, J. Foster

2:30 POLY **320.** New strategies for polymer functionalization: From multifunctional homopolymers to polymeric thermometers. C.A. Figg, T. Kubo, R.N. Carmean, C.P. Kabb, **B.S. Sumerlin**

3:00 Intermission.

3:20 POLY **321.** Cyclopolymerization using Grubbs catalyst. **T. Choi**

3:40 POLY **322.** Carbohydrate-based macromolecular self-assemblies and their biological functions. **G. Chen**

4:00 POLY **323.** Harnessing non-covalent interactions for functional organic and polymeric materials. **L. Fang**, T. Yuan, C. Zhu, M.A. Olson

4:20 POLY **324.** Functional materials constructed by the combination of traditional polymers and host-guest molecular recognition motifs. **F. Huang**

Polymers under Deformation

Applying Advances in Characterization Methods for In-Situ Studies of Deformation

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Advances in Polysaccharides: Practice & Applications

New Developments in the Industrial Sector

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Recent Advances in Multiblock Copolymers

Synthesis & Modeling

Sponsored by PMSE, Cosponsored by POLY‡

TUESDAY EVENING

Section A

Moscone Center

Hall A

Excellence in Graduate Polymer Research

Cosponsored by PRES, PROF, SOCED and YCC

Financially supported by POLY Industrial Advisory Board

H. Cheng, C. J. Ellison, C. J. Landry-Coltrain, T. E. Long, *Organizers*

6:00 - 8:00

POLY **325.** Diversifying catalysts, monomers, cross-coupling strategies and functional groups in the controlled synthesis of conjugated polymers. **Y. Qiu**, K.J. Noonan, T. Kowalewski

POLY **326.** Bioinspired stimuli-responsive materials: Concurrent shape and color change in programmed cholesteric liquid crystal elastomers. **M.T. Leslie**, G.E. Wnek, L.T. Korley, T.J. White

POLY **327.** Towards commercially scalable processes for polymers produced by sequential anionic and RAFT polymerization. **M. Forrester**, W. Bradley, N. Hernandez, G.A. Kraus, E.W. Cochran

‡ *Cooperative Cosponsorship*

POLY **328.** Scalable synthesis of macroCTAs from living anionic polystyrene. **W. Bradley**, M. Forrester, N. Hernandez, G.A. Kraus, E.W. Cochran

POLY **329.** Synthesizing Hyperbranched Polyglycerol (HPG) derivatives for use in templating hard inorganic nanostructures, biocompatible soft nanoparticles and structure-preserving binder materials for batteries. **J. Iocozzia**, Z. Lin

POLY **330.** Synthesis of biodegradable polycarbonate nanostructures with selective lysis against gram positive bacteria. A**. Nimmagadda**, J. Cai

POLY **331.** Promising approach to developing eco-friendly, sustainable and dual-cure coatings. **O. Akdogan**

POLY **332.** Engineering zwitterionic polymers that control cell adhesion and direct neurite growth to improve cochlear implants. **B. Leigh**, E. Cheng, M.R. Hansen, A. Guymon

POLY **333.** Modification of alkene-containing copolylactide scaffolds for biomedical applications. **P. Kalelkar**, R. Agarwal, A. Garcia, D.M. Collard

POLY **334.** Chalcogen polymers for completely solution-processed inorganic photovoltaics. **T.R. Martin**, H. Hillhouse, C.K. Luscombe

POLY **335.** Fluorinated thiophenes in PBnDT-TAZ for bulk heterojunction solar cells: The impact of fluorination. **Q. Zhang**, L. Yan, W. You

POLY **336.** Introducing cobaltocenium to Alkaline Anion Exchange Membrane Fuel Cells (AAEMFC). **H. Yuan**, T. Tsai, B. Coughlin

POLY **337.** Real-time metrology for photopolymer additive manufacturing with exposure controlled projection lithography. **X. Zhao**, D.W. Rosen

POLY **338.** Nanoscale considerations responsible for diverse macroscopic phase behavior in substituted isobutyl-POSS/poly(ethylene oxide) blends. **Y. Caydamli**, E. Yildirim, J. Shen, X. Fang, M.A. Pasquinelli, R.J. Spontak, A.E. Tonelli

POLY **339.** Stable entrapment of cholesteric 1D photonic domains in Liquid Crystalline Random Terpolymer (LCRTP) architecture with dual covalent and physical networking sites: A platform towards elastomeric 1D photonic material. **L.H. Mahajan**, D. Ndaya, P.B. Deshmukh, M. Gopinadhan, C.O. Osuji, R. Kasi

POLY **340.** Nanoporous materials from ultrahigh molecular weight linear block copolymer precursors. **J. Mapas**, J. Rzayev

POLY **341.** Segmental dynamics of poly(styrene-stat-methyl methacrylate-d_3) in bulk and at very small amounts on silica. **U.N. Arua**, M. Madduma Arachchilage, F.D. Blum

POLY **342.** Simple and accurate determination of reactivity ratios of chain copolymerization following terminal model by *in-situ* ^{1}H-NMR technique. **D. Debnath**, J. Baughman, R.A. Weiss, C.R. Pugh

POLY **343.** Withdrawn.

Section A

Moscone Center
Hall A

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

6:00 - 8:00

POLY **344.** Effect of organically modified montmorillonite on polymerization and thermal degradation mechanisms of polybenzoxazine. **A. Hisar Telli**, J. Hacaloglu

POLY **345.** Hydrophilic-hydrophobic hydrid polymer involving perfluoro- with tetraarylphosphonium moieties: Synthesis, film morphology and electrochemical properties. **W. Wan**, X. Yang, R. Smith

POLY **346.** CdSe/CdS-Conjugated polymer core-shell hybrid nanoparticles by a grafting-from approach. **S. Huber**, T. Deroo, D. Seletskiy, A. Leitenstorfer, S. Mecking

POLY **347.** Anisotropic nanocrystals from precisely long-spaced ionomers. **C. Rank**, S. Mecking

POLY **348.** Dual-patterning optical data storage in polymer films with orthogonally responsive dyes. **P. Wei**, B. Li, A.D. Leon, E. Pentzer

POLY **349.** 2,1,3-Benzooxadiazole, thiophene and benzodithiophene based random copolymers for organic photovoltaics: Thiophene versus thieno[3,2-b]thiophene as π-conjugated linkers. **S. Goker**, G. Hizalan, E. Aktas, S. Kutkan, A. Cirpan, L. Toppare

POLY **350.** Multifunctional phosphorus flame retardants for polymeric materials from benzoquinone. **A. Alrubayyi**

POLY **351.** Photochemical controlled dissulfide based thiol-ene/thiol-Michael covalent adaptable network development and application. **X. Han**, X. Zhang, N. Sowan, L. Cox, S. Huang, C. Bowman

POLY **352.** Withdrawn.

POLY **353.** Oligomeric 3,4-propylenedioxythiophene dyes for achieving color neutrality with electrochromic devices. **O.A. Yassin**, M.T. Otley, X. Zhang, M. Li, G.A. Sotzing

POLY **354.** In-situ stabilization of polyolefins in aqueous systems by inorganic particles. **T. Morgen**, S. Mecking

POLY **355.** Structure-property relationships of conjugated polymers. **S.S. Lawton**, D.M. Haddleton

POLY **356.** Fluorinated polymethacrylate bottlebrush enables outstanding water- and oil-repellent surfaces. **Y. Luo**, K. Hong

POLY **357.** Phosphonate functionalized poly-3-hexylthiophenes by controlled Suzuki-Miyaura coupling polymerization for interface modification in hybrid solar cells. **A. Groh**, P. Ehrenreich, L. Schmidt-Mende, S. Mecking

POLY **358.** Triplet-Triplet annihilation upconversion in epoxy-amine networks. **A.K. Williams**, J. Lott

POLY **359.** Flexible sulfur copolymr film via inverse vulcanization technique. V. Wadi, S. Khawaja, **S. Al Hassan**

POLY **360.** Syntheses, electrochemical and spectroelectrochemical characterizations of quinoxaline-based conjugated polymers for organic photovoltaics. **M. Yasa**, S. Goker, Y. Arslan Udum, G.E. Gunbas, L. Toppare

POLY **361.** Analysis of polyamides with GPC using triple detectors. **R. Farasat**

POLY **362.** Rapid screening of packaging for residual monomers using SIFT-MS. V.S. Langford, **B.J. Prince**, D.B. Milligan, M. Perkins, T. Wilks, T. Potter

POLY **363.** FTIR characterization of co-deposited LbL film of sPPO and sPS copolymer with PDDA. **C.G. Cho**, H. Ryu, A. Heo

POLY **364.** Polysulfone-poly(diallypiperidinium hydroxide) multiblock copolymers containing alkaline stable spirocyclic quaternary ammonium cations for alkaline exchange membranes. **B.J. Graziano**, D.J. Strasser, D.M. Knauss

POLY **365.** Investigating the dynamic assembly of boronate esters and diazaboroles for the formation of frameworks and polygons. **V. Drogkaris**, B.H. Northrop

POLY **366.** Withdrawn.

POLY **367.** Structure-property-processing-application relationship of amino acid-based poly(ester urea)s. **J. Yu**, M. Becker

POLY **368.** From exhaust gas to drug delivery: Nano carriers based on carbon dioxide and tailored epoxide building blocks. **M. Scharfenberg**, H. Frey

POLY **369.** Hyperbranched polymers for the disruption of quorum sensing in pseudomonas aeruginosa. **W. Martin**, J. Shepherd

POLY **370.** Smart polymers - drug delivery with polyvinylphosphonates. **C. Schwarzenböck**, B. Rieger

POLY **371.** Polyglutamic acid based GRAS nanogels for drug delivery. **P. Prasad**, M. Molla, W. Cui, M. Canakci, B. Osborne, J. Mager, S. Thayumanavan

POLY **372.** Conformational effect of trehalose monomers and polymers on protein stabilization. **M. Messina**, J. Ko, Z. Yang, J.M. Strouse, K.N. Houk, H.D. Maynard

POLY **373.** Fabrication of biodegradable surfaces of modified poly(-lactic acid) for biomedical applications. **P. Kalelkar**, D.M. Collard

POLY **374.** Investigation of the dynamic aminal bond exchange towards the design and synthesis of polyaminal polymers. **A. Chao**, D. Zhang

POLY **375.** Bio-based semi-crystalline polyphosphoesters *via* polyesterification reactions. **H. Busch**, S. Mecking

POLY **376.** Encoding function in protein-oligonucleotide precision biopolymers. **W. Liu**, T. Weil

POLY **377.** Poly(acrylic acid) based block copolymers as excipients for enhancing solubility of poorly water soluble drugs. **A. Purchel**, W.S. Boyle, T.M. Reineke

POLY **378.** Dual effect of thiol addition on fluorescent polymeric micelles: ON-to-OFF emissive switch and morphology transition. **A.B. Mabire**, M. Robin, H. Willcock, A. Pitto-Barry, N. Kirby, R.K. O'Reilly

POLY **379.** Fabrication and orthogonal modification of multi-functional nanogels for targeted therapy. **L. Chambre**, B. Aktan, R. Sanyal, A. Sanyal

POLY **380.** Withdrawn.

POLY **381.** Catalytic precision polymerization of polar monomers: Rare earth metal-mediated synthesis of homopolymers and polymer brushes. **P. Pahl**, B.S. Soller, B. Rieger

POLY **382.** High swelling acrylate elastomers with a RAFT crosslinker by high-throughput approach. **J. Lee**, K.A. Cavicchi

POLY **383.** Amino functional poly(propylene oxide). **J. Blankenburg**, J. Herzberger, H. Frey

POLY **384.** Novel aliphatic polycarbonate elastomers based on CO_2 and epoxides. **L. Kunze**

POLY **385.** Synthesis of star-comb double crystalline copolymers of ε-caprolactone /$_L$-lactide: Effect of main-chain structure on crystallization behavior. **X. Leng**

POLY **386.** Diene functional polyethers: A versatile platform for triazolinedione click chemistry: New multi-functional PEGs for pharmaceutical purposes and clickable polyethers. **T. Johann**, H. Frey

POLY **387.** Advances in Pd-initiated polymerization of diazoacetates: From variety of functional groups, living polymerization system, to high stereoregularity. **H. Shimomoto**, E. Ihara

POLY **388.** One-Pot synthesis of hyperbranched polymers with over a million molecular weight and low polydispersity. **X. Cao**, Y. Shi, X. Wang, R. Graff, H. Gao

POLY **389.** Safrole Oxide (SFO): A novel functional epoxide monomer for the introduction of Catechol moieties into multifunctional Poly(ethylene glycol) via monomer activated technique. **O. Linker**, T. Johann, H. Frey

POLY **390.** Withdrawn.

POLY **391.** Chain multiplication of fatty acids. **M. Haeussler**, T. Witt, S. Mecking

POLY **392.** Synthesis and applications of dialkyne functionalized fulvenes. **A. Peloquin**, N.P. Godman, G.J. Balaich, S.T. Iacono

POLY **393.** Side group effects on aggregation properties of conjugated polymers. **Y. Yang**, K.S. Schanze

POLY **394.** Synthesis of DABCO based cationic polymers with ROMP technique and examination of antibacterial activity. **A. Kaymaz**, T. Eren, S. Bucak

POLY **395.** Click chemistry toward stable reverse osmosis membranes for water desalination. **B.L. Hamlett**, M. Finn, R.P. Lively, B. McCool

POLY **396.** Synthesis of high melting precision aliphatic polysulfones via ADMET polymerization. **M.H. Bell**, G. Hester, T.W. Gaines, K.B. Wagener

POLY **397.** Self-Assembly of brush block copolymer photonic crystals featuring low T_g side chains. **A.L. Liberman-Martin**, C. Chu, A. Chang, R.H. Grubbs

POLY **398.** Synthesis of molecular brushes with ultrahigh grafting density using accelerated CuAAC coupling-onto strategy. **Y. Shi**, W. Gan, X. Cao, H. Gao

POLY **399.** Ultra-rigid indenyl-based group IV metallocene complexes for nearly perfect ^{i}PP catalysis. **M. Machat**, B. Rieger

POLY **400.** Controlled ring-opening polymerization of *O*-carboxyanhydrides using β-diiminate zinc catalyst. **R. Wang**, J. Cheng

POLY **401.** Microwave-assisted polyarylene: Synthesis, characterization, and optimization. **S.M. Budy**, D.Y. Son

POLY **402.** Expanding the scope of radical traps in RTA-ATRC reactions by using solvent mixtures and additives. **E.S. Tillman**, **M. Arce**

POLY **403.** Withdrawn.

POLY **404.** High-strain elastomeric networks from thiol-ene chemistry. **A.J. Guenthner**, J.C. Marcischak, T.S. Haddad, J. Reams, M.D. Ford, J.M. Mabry

POLY **405.** Synthesis of polythiophene as a possible smart functional polymer. **M.N. Siddiqui**, N. Ullah, A. Al-Betar, A. Al-Saadi

POLY **406.** Synthesis and characterization of multi-cationic quaternary ammonium containing polymers. **Z.D. Whitermore**, S.M. Duggan, M.C. Jennings, W.M. Wuest, K.P. Minbiole, D.L. Zubris

POLY **407.** Withdrawn.

POLY **408.** Computational and experimental investigations of the thiol-Michael click reaction and its applications in dendrimer synthesis. **S.H. Frayne**, B.H. Northrop

Section A

Moscone Center

Hall A

Polymer Applications & Characterization in the Biomedical Industry

X. M. Liu, J. Slager, *Organizers*

6:00 - 8:00

POLY **409.** ^{1}H NMR study on polymer-peptide mixed micelles for adjuvant application. **O. Zholobko**, A. Kohut, A.S. Voronov

POLY **410.** Delivering antigen to monocytes using protein transduction domain mimics. **C. Backlund**, G.N. Tew, T.L. Andresen, L. Parhamifar

POLY **411.** Polymer structure and conformation alters immune recognition of viral nanoparticle-polymer conjugates. **P. Lee**, S. Isarov, J.D. Wallat, P. Stewart, N. Steinmetz, M.J. Hore, J.K. Pokorski

POLY **412.** Polymeric HIPE foams as multifunctional wound dressings designed for treatment of combat-related trauma. **C.L. McGann**, B. Streifel, J. Lundin, J.H. Wynne

POLY **413.** Genomic DNA functionalized architected materials fabricated via two-photon lithography for drug capture. **D. Yee**, M.D. Schulz, C. Blumenfeld, R.H. Grubbs, J.R. Greer

POLY **414.** Rheological characterization of alginate-based hydrogels for biomedical applications. **W. Hom**, S.R. Bhatia

POLY **415.** Microcomputed tomography study of the wear behavior of porous PEEK for spine devices. **D. Safranski**, N. Evans, B. Torstrick, A. Lin, K. Gall, R.E. Guldberg

POLY **416.** Withdrawn.

POLY **417.** Sandcastle worm-inspired blood-resistant bone graft binder using a sticky mussel protein for augmented *in vivo* bone regeneration. **H. Kim**, B. Choi, H.J. Cha, S. Jun

POLY **418.** Protein stabilization via Poly(Ethylene Glycol)-based (PEG) amphiphilic nanomicelles. **Y. Lien**, M.R. Smith

POLY **419.** Brushed polymers as promising grafting agents against protein binding. **B. Wang**, T. Blin, A. Käkinen, X. Ge, E. Pilkington, J. Quinn, M. Whittaker, T. Davis, P. Ke, F. Ding

POLY **420.** Charge-Altering Releasable Transporters (CARTs) for the delivery and release of messenger RNA in living animals. **C. McKinlay**, J. Vargas, T. Blake, J. Hardy, K. Masamitsu, C. Contag, P.A. Wender, R.M. Waymouth

Section A

Moscone Center

Hall A

Polymeric Materials for Performance & Sustainability

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

6:00 - 8:00

POLY **421.** Organic solar cell based on porphyrin functionalized Rosette nanotube. **E. Keyvani-Someh**, L. Shuai, W. Lee, H. Fenniri

POLY **422.** Synthesis and applications of recyclable polymer-bound transition metals sequestrants. **D. Chouikhi**, T. Malinski, M. Al-Hashimi, D.E. Bergbreiter, H.S. Bazzi

POLY **423.** Cross-linked films from star-shape poly(ε-caprolactone): Effects of branch number and chain length on elastic properties. **D.K. Saha**, M. Ebara, T. Aoyagi

POLY **424.** Effects of molecular weight on power conversion efficiency of an end-capped polythiophene. **P.R. Pulley**, D.J. Patterson

POLY **425.** PHB and Montmorillonite Clay Composites as KNO_3 and NPK controlled release fertilizers. J. Souza, A. Campos, **R. Faez**

POLY **426.** Chitosan-montmorillonite spray dried microsphere and microcapsules for fertilizer encapsulation. D. França, Â.F. Medina, C.F. Souza, **R. Faez**

POLY **427.** Nontoxic and nonvolatile alternatives for hexane and heptane and their use in catalysis. **M.L. Harrell**, T. Malinski, C. Torres-Lopez, K. Gonzalez, D.E. Bergbreiter

POLY **428.** Sustainable polyaldimines from lignin-derived aromatic aldehydes and aliphatic diamines. **M. Rostagno**, S.A. Miller

POLY **429.** High performance waterborne exterior coatings with improved durability, eco-footprint and cost through the use of self-assembled polymer pigment composites. **J. Bohling**, P. Luo, J. Tanzer, A.M. Maurice, M. Koback, M. Belowich, C. Valente, W. Gao, J. Reffner

POLY **430.** Succinate polyester polyol copolymers and blends: Synthesis, compatibility, crystallization kinetics, and crystal morphologies. **H.S. Hamilton**, **A.A. Seba**, **J.E. Blue**, W.D. Coggio, A. Schrock

POLY **431.** Novel conjugated polymer binders and their processing for Si-based Li-ion battery anodes. **A.L. Miranda**, X. Li, H. An, J.L. Lutkenhaus, R. Verduzco

POLY **432.** Aniline oligomers and polyaniline: Supercapacitors and freestanding films. **C. Lin**, R. Li, R.B. Kaner

POLY **433.** Exploring inverse vulcanization of sulfur with natural source monomers as cathodic materials for long life lithium sulfur batteries. **I. Gomez**, O. Leonet, A. Blazquez, D. Mecerreyes

POLY **434.** Synthesis and properties of physically cross-linked hydrogel obtained from amphiphilic copolymer. **D. Debnath**, R.A. Weiss, C.R. Pugh

POLY **435.** Effects of substituents on the ceiling temperature of cyclopentene in ring-opening metathesis polymerization. **H. Liu**, Y. Ren

POLY **436.** Periodical mesoporous polymers from H-bonding-modulated block copolymer supramolecules. **Y. Wang**, **L. Guo**

POLY **437.** Photo-responsive solubility, color, and fluorescence of phthalocyanine dye in solution and polymer films. **B. Li**, P. Wei, A. de Leon, T. Frey, E. Pentzer

POLY **438.** New achievement toward greener BIAN-NHC ruthenium complex. **A.R. Hlil**, J. Balogh, R. Tuba, M. Al-Hashimi, H. Bazzi

POLY **439.** Thiol-ene polymerization of biobased monomers deriving from syringaresinol. Y. Chen, M. Janvier, S. Jaufurally, P. Ducrot, **F. Allais**

POLY **440.** Effect of methoxy substituent position on thermal properties and solvent resistance of lignin-inspired poly(dimethoxy phenyl methacrylate). **S. Wang**, G. Wieber, T.H. Epps

POLY **441.** Improving the rheology and mechanical response in alumina-poly(vinylidene fluoride)-poly(lactic acid) composites. **J. Bencomo**, J.M. McCollum, S.T. Iacono

Section A

Moscone Center

Hall A

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Cosponsored by PMSE

D. H. Thompson, G. Wenz, *Organizers*

6:00 - 8:00

POLY **442.** Self-healing hydrogels based on ionic interactions and host-guest complexation using both cationic β-cyclodextrin oligomers and anionic poly(acrylic acid) networks. **S. Joo**, D. Jeong, S. Jung

Section A

Moscone Center

Hall A

Structure to Function in Supramolecular Polymers & Materials

P. Besenius, R. Kieltyka, J. B. Matson, *Organizers*

6:00 - 8:00

POLY **443.** Thermodynamic insights into the entropically driven self-assembly of rylene bisimide dyes in water. **P. Peethambaran Nair Syamala**, D. Goerl, B. Soberats, F. Wuerthner

POLY **444.** Kinetic control of supramolecular polymerization by ultrasonication. **M. Wehner**, S. Ogi, W.J. Wagner, V. Stepanenko, F. Wuerthner

POLY **445.** Molecular weaving of flexible covalent organic frameworks. **Y. Liu**, Y. Ma, O. Terasaki, O.M. Yaghi

POLY **446.** Unique dynamics of poly(dimethyl siloxanes) with associating chain ends. **K. Xing**, P. Cao, M. Tress, T. Saito, V. Novikov, S. Cheng, A.P. Sokolov

POLY **447.** Structure and rheology of hydrophobic modified polyacrylamide-nanoparticle mixture. **F. Peng**, Y. Ke

POLY **448.** Heparin-Treated trehalose-based polymers exhibit ehanced transfection efficiency in challenging cell types. **W. Boyle**, T.M. Reineke

Section A

Moscone Center

Hall A

Undergraduate Research in Polymer Science

J. Lott, S. E. Morgan, S. I. Nazarenko, *Organizers*

6:00 - 8:00

POLY **449.** Design and synthesis of solution processable *n*-channel π-conjugated polymers and device applications. **A. Tonnaer**, R. Topiwala, N. Patel, Z. Yuan, E. Reichmanis

POLY **450.** Novel copolymers of styrene and some ring-disubstituted propyl 2-cyano-3-phenyl-2-propenoates. **G.B. Kharas**, V.A. Sloan-Lyon, M. Cieszynski, J.D. Manuel, S.L. Mei, J.B. Mubang, P.E. Skorseth, K.E. Smith, N. Tassone, E. Tolberd, D.Z. Yan

POLY **451.** Fabricating novel optical sensors by embedding gold nanoparticles inside peptoid nanosheets. **K. Chen**, E. Robertson, R.N. Zuckermann

POLY **452.** Exploration of the electron transfer reaction between 1-ethyl-3-methyl-4-vinyl imidazolium triflate and ethyl vinyl ether. **S. Lucisano**, M. Detwiler, T.W. Smith

POLY **453.** Synthesis, characterization and photophysical properties of new 2-(2-methoxyphenoxy)-6-(3-methoxyphenoxy)-1,5-naphthyridine):phenylene vinylenes copolymers. **A.A. Boali**, M. Mansha, N. Ullah

POLY **454.** Synthesis and characterizaiton of conducting polymers with degradable crosslinks. **R. Grant**, A. Murphy

POLY **455.** Actuation of electrospun silk-conducting polymer composites. **J. Bontrager**, T. Fuller, S. Maxwell, A. Murphy

POLY **456.** Solvent effects and isothermal crystallization of poly(ethylene oxide)-block-poly(ε-caprolactone). **C. Tower**, R.M. Van Horn, K. Allen, A. Carandang

POLY **457.** Crystallization trends of equal molecular weight poly(ethylene oxide)-*b*-poly(caprolactone). **N. Brigham**

POLY **458.** Isothermal crystallization analysis of poly(ethylene oxide)-block-poly(ε-caprolactone) with Larger w_{PEO} or w_{PCL}. **M. Steffen**, R.M. Van Horn

POLY **459.** Synthesis of low molecular weight anionic acrylamide-based polymers for determination of structure/binding onteractions with α-gliadin. **H. Kolell**, A. Bristol, S.E. Morgan

POLY **460.** Amine assisted photo-initiated RAFT polymerization using visible light: A kinetic and mechanistic study. M. Allegrezza, Z. DeMartini, A. Kloster, **Z. Digby**, D. Konkolewicz

‡*Cooperative Cosponsorship*

POLY **461.** Employment of thiazolidine chemistry for novel polymer composition and structure. **C. DeHoe**, C. Sarantes, K. Eckhart, L. Souza, P.J. Costanzo

POLY **462.** Characterization of a thiol-ene/acrylate-based polymer for neuroprosthetic implants. **D. Do**, M. Ecker, W. Voit

POLY **463.** Withdrawn.

POLY **464.** Highly functional methacrylated bio-based resin system for UV/Vis-curable coatings. **J. Sahouani**, A.Z. Yu, D.C. Webster

POLY **465.** Finding green alternatives to platinum catalysts for the hydrosilylation and hydrogenation of carboxylic acid derivatives. **J. Arens**, C. Cheng

POLY **466.** Synthesis and characterization of highly fluorinated dendrimers utilizing orthogonal chemistry. **A. Richert**, A.R. Jennings, S.T. Iacono

POLY **467.** Molecular weight changing polymers via Diels-Alder chemistry. **T. Schoch**, M.R. Martinez, M. Meyersohn, M. Markmann, **P.J. Costanzo**

POLY **468.** Thio-bromo click approach for the preparation of a new class of cross-linked, ROMP-based gels. **D. Gutierrez**, C.E. Hobbs

POLY **469.** Inversion of molecular topology and composition using Diels-Alder chemistry. **M. Meyersohn**, M. Markmann, **P.J. Costanzo**

POLY **470.** Gallic acid esters with flame retarding properties. **K.L. Oberdorfer**

POLY **471.** Magnetic field triggered degradation of xylan with a xylanase-copolymer conjugate for controlled drug delivery. **T. Richardson**

POLY **472.** Development of new fluorocyclic-polyhedral oligomeric silsesquioxane containing polymers of varying architectures. **E.C. Lochmaier**, A.R. Jennings, S.T. Iacono

POLY **473.** Amphiphilic polyurethane coatings for fouling release applications. **R. Burgett**, D.C. Webster, T.P. Galhenage

POLY **474.** Oligomeric flame retardants for polymeric materials from itaconic acid. **V. Hill**, B. Howell, Y. Daniel

POLY **475.** Polysoaps to serve as stimuli-responsive micelles for environmental remediation applications. **C.R. Kasprzak**, P.D. Pickett, C.L. McCormick

POLY **476.** Counterion effects on the glass transition temperature of ionic liquid polymers. **A. Mayers**, S. Lucisano, T.W. Smith

POLY **477.** Ab initio Monte Carlo simulations of military contaminants binding to cellulose and its derivatives. **T. Truttmann**, M. Roth, G. Todde, M.K. Shukla, G. Subramanian

POLY **478.** Reducing immune response of nucleic acids by brush polymer assisted compaction. **M. Corley**, X. Lu, X. Cao, K. Zhang

POLY **479.** Nanomorphology of novel synthesized diblock copolymers with and without lithium salt characterized by atomic force microscopy. **M. Longstaff**, D.A. Waldow

POLY **480.** Time-Dependent release of methylene blue from PEO-*b*-PCL films for the prevention of anaphylaxis. **H. Fischer**, J.E. Jurczyk, M. Seraly, R.M. Van Horn

WEDNESDAY MORNING

Section A

Moscone Center
120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

B. M. Aden, A. Shete, *Presiding*

8:00 POLY **481.** Synthesis and fabrication of Persistent Micelle Templates (PMT) in a single day. **A. Sarkar**, M. Stefik

8:20 POLY **482.** Rapid free-electron initiated selective polymerization at room temperature. **B. Chang**, S. Oyola-Reynoso, J. Chen, M. Lu, M. Thuo

8:40 POLY **483.** Blue-light activated bulk photo-Cu(I)-catalyzed azide-alkyne cycloaddition (photo-CuAAC) click reaction-based networks: Properties and application. **A. Shete**, B. El-Zaatari, C.J. Kloxin

9:00 POLY **484.** Aza-Michael reaction applied to PDMS: Kinetic modelling, selectivity control and novel potentialities. A. Genest, S. Binauld, E. Pouget, F. Ganachaud, E. Fleury, **D. Portinha**

9:20 POLY **485.** Stereoregular copolymerization of butadiene with heterofunctionalized diene monomers. **I. Goettker Genannt**, H. Leicht, S. Mecking

9:40 POLY **486.** Investigations on polystyrene – C60 nanocomposites. **E. Ibrahim**, S. Casas, D. Chipara, J. Hinthorne, M. Chipara

10:00 POLY **487.** In situ gradient functionalization of azlactone-based block copolymer brushes. **B.M. Aden**, B.S. Lokitz, M. Kilbey

10:20 POLY **488.** Improvement of nitinol corrosion resistance by SiATRP: The key role of electrografting process. B. Arrotin, J. Delhalle, P. Dubois, Z. Mekhalif, **L.M. Mespouille**

10:40 POLY **489.** Zwitterionic diblock copolymer nanoparticles prepared by polymerization-induced self-assembly exhibit pH-responsive schizophrenic behavior. **S.L. Canning**, S.P. Armes

11:00 POLY **490.** Poly(S-alkylsulfonylcysteines): The first cysteine derivatives combining stability during polypeptide synthesis with fast chemoselective disulfide formation. **M. Barz**

11:20 POLY **491.** Bio-Based oligoethers from isosorbide and 1.3-propanediol: Synthesis and characterization. **E. Fleury**, J. Rodier, A. Rousseau

Section B

Moscone Center
121

Next Generation Smart Materials

Cosponsored by MPPG‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

M. Karman, J. Lott, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **492.** Bioinspired control of polymer self-assembly via ligand-metal ion interactions. **A. Knight**, J. Larsson, C.J. Hawker

8:25 POLY **493.** Let's get things in order: Sequence controlled anionic polymerization of aziridines. **E. Rieger**, T. Gleede, A. Manhart, L. Thomi, M. Wagner, F. Wurm

8:45 POLY **494.** Design and synthesis of cellulose based polyelectrolytes via olefin cross-metathesis. **B.L. Nichols**, K.J. Edgar

9:05 POLY **495.** Hollow polycaprolactone nanocages from variable grafting-density polymer-grafted silica nanoparticles: Materials for next-generation oil dispersants. **K.C. Bentz**, M. Ejaz, S.M. Grayson, D. Savin

9:25 POLY **496.** Group-Transfer-Polymerization: A highly versatile tool for tailor-made smart polymers. **F. Adams**, P.T. Altenbuchner, B. Rieger

9:45 Intermission.

9:55 POLY **497.** Smart hydrogel-based valves inspired by the stomata in plants: Ability to regulate water flow based on temperature, pH, and light. **S.R. Raghavan**, A. Gargava

10:15 POLY **498.** Design and study of biodegradable and photodegradable thermoplastic elastomers. **K.J. Arrington**, J. Waugh, S. Radzinski, J. Matson

10:35 POLY **499.** Stimuli-Responsive dendronized polymers for next generation biomaterials. **W. Li**, J. Yan, K. Liu, A. Zhang

10:55 POLY **500.** Smart organic two-dimensional materials based on a rational combination of non-covalent interactions. **J. Ziwen**, W. Bai, S. Thayumanavan

11:15 POLY **501.** Discrete chromophores as a path towards high contrast anodically coloring electrochromic polymers. **D. Christiansen**, A.L. Tomlinson, J.R. Reynolds

Section C

Moscone Center
122

Polymeric Materials for Performance & Sustainability

Other Functional Materials

Cosponsored by MPPG‡

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

R. L. Snyder, *Presiding*

8:00 POLY **502.** Synthesis and evaluation of thermally-responsive coatings based upon Diels-Alder chemistry and renewable materials. D. Amato, G. Strange, J.P. Swanson, K. Varney, D. Amato, **P.J. Costanzo**

8:30 POLY **503.** Superhydrophobic nanocomposite films based on polypentafluorostyrene-modified fumed silica. **Q. Yin**, E. Beyou, A. Charlot, D. Portinha

8:50 POLY **504.** Environmentally-safe and transparent superhydrophobic coatings. **J. Mates**, R. Ibrahim, A. Vera, S. Guggenheim, J. Qin, D. Calewarts, D. Waldroup, C. Megaridis

9:20 POLY **505.** Polyelectrolyte multilayer nanocoating exhibiting super oxygen gas barrier and 100% self-healing efficiency. **Y. Song**, K. Meyers, R. Ramakrishnan, J. Gerringer, S. Qin, M. Humood, S.I. Nazarenko, J.C. Grunlan

9:40 Intermission.

9:55 POLY **506.** Polyphenylenesulfide and polyetheretherketone POSS nanocomposites: Improvements in rheological and crystallization behavior. **S.E. Morgan**, K.M. Knauer, G. Brust, M. Carr, R. Cardona, J. Lichtenhan

10:25 POLY **507.** Carbon nanofiber and graphene nanoplatelet containing polycaprolactam nanocomposites: Improvements in mechanical performance in the context of unique interfacial interactions. **J. Buchanan**, E.R. Reed-Gore, S.L. Williams, Z.B. McClelland, R.D. Moser, M.K. Shukla

10:55 POLY **508.** Robust and scalable macromolecular architectures as additives for lubrication oils. **R. Bou Zerdan**, B. van Ravensteijn, D. Seo, N. Cadirov, D. Lee, J. Gerbec, T. Watanabi, C.J. Hawker, M.E. Helgeson, J.N. Israelachvili

Section D

Moscone Center
123

Polymers & Biomimicry

A. N. Dhinojwala, T. Williams, *Organizers*, *Presiding*

8:00 POLY **509.** Natural and bioinspired polyphenols as multifunctional coatings. **P.B. Messersmith**, P. Burch, W. Reese, K. Healy

8:30 POLY **510.** Designing mechano-responsive polymers that encompass biomimetic cryptic bonds. S. Biswas, V. Yashin, **A. Balazs**

8:50 POLY **511.** Host-defense peptide-mimetic polymers to target the solution state of bacteria for modulation of biofilm formation. **L. Foster**, S.I. Yusa, K. Kuroda

9:10 POLY **512.** Polymerization in micro channels of teeth towards artificial leaves. **J.C. Tiller**, C. Fik

9:30 POLY **513.** Effects of *Stenocara* beetle-inspired biphilic patterns on the rate of water collection from humid air. **J.J. Benkoski**, K. Gerasopoulos, L. Luedeman, M. McCarthy, M.M. Rahman, E. Ölçeroglu

9:50 Intermission.

10:05 POLY **514.** Effects of chemistry and dynamic three dimensional morphology of the epicuticular wax on water wettability and permeability of the prickly pear cacti cuticle. **K. Rykaczewski**, R. Linder, K. Manning, L. Majure

10:35 POLY **515.** Mimicking muscle fiber structure and function through electromechanical actuation of nanofiber bundles. S.Y. Severt, S. Maxwell, J. Bontrager, T. Fuller, J. Leger, **A. Murphy**

10:55 POLY **516.** Advances in asymmetric heterogeneous catalysis: Synthesis of novel nanoreactors. **E. Lestini**, L.D. Blackman, R.K. O'Reilly

11:15 POLY **517.** Rational design of antifreeze-protein mimetic materials to enable the cryopreservation of cells. **M.I. Gibson**

11:35 POLY **518.** Biomimetic polymer coated carbon nanotube gas sensor for real-time air quality sensor suite. Y.H. Ngo, G. Slusher, K. Fullerton, C. Suarez, R.R. Naik, J.A. Martin, C. Grigsby, **S.S. Kim**

Section E

Moscone Center
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Structure to Function in Supramolecular Polymers & Materials

R. Kieltyka, *Organizer*

P. Besenius, J. B. Matson, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **519.** Self-assembly and hydrogelation of a peptide derived from semenogelin I. **K.S. Akerfeldt**

8:30 POLY **520.** Tubular supramolecular polymers. **H. Cui**

8:55 POLY **521.** Withdrawn.

9:15 POLY **522.** Light-triggered self-assembly and actuation of DNA nanostructures using photocaged nucleotides. **N. Stephanopoulos**

9:40 Intermission.

9:55 POLY **523.** Supramolecular materials from virus-like particles as building blocks. **J.J. Cornelissen**

10:20 POLY **524.** Supramolecular gels for delivery of hydrogen sulfide. **J.B. Matson**, Y. Qian, K. Kaur

10:45 POLY **525.** Tubular supramolecular polymers. **S. Perrier**

11:10 POLY **526.** Synthesis of a tough thermoplastic elastomer that rapidly absorb water for use in hemorrhage control applications. **T.R. Long**, E. Bain, F.L. Beyer, R. Mrozek, A.M. Savage, J. Lenhart

11:30 POLY **527.** Functional, bio-inspired supramolecular polymeric materials – the interplay between covalent and non-covalent bonds. O. Goor, M. Grillaud, P. Fransen, **P.Y. Dankers**

Section F

Moscone Center

125

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Self-Healing Materials & Networks

Cosponsored by PMSE

Financially supported by Wacker Chemical Corporation, Jewell Laboratories LLC

D. H. Thompson, *Organizer*

G. Wenz, *Organizer, Presiding*

A. E. Tonelli, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **528.** From synthesis of nonlinear block copolymers based on cyclodextrins to functional nanoparticles and Shish-Kebabs. **Z. Lin**

8:35 POLY **529.** Slide-Ring materials: Tough polymers from cyclodextrin. **K. Ito**

9:05 POLY **530.** Supramolecular materials: Self-healing and stimuli-responsive polymeric materials through host-guest interactions. **A. Harada**

9:35 Intermission.

9:50 POLY **531.** Peculiar viscoelasticity and tensile behavior of polyrotaxane glass. **K. Kato**, K. Nemoto, K. Mayumi, H. Yokoyama, K. Ito

10:20 POLY **532.** Self-healing car paints from cyclodextrin polyrotaxanes. **G. Wenz**, G. Kali

10:50 POLY **533.** Concurrent covalent and supramolecular polymerization. X. Hou, C. Ke, **J.F. Stoddart**

11:20 Panel Discussion.

Bio-based Gels & Porous Materials

Biopolymer Hydrogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Polymers under Deformation

AFM & Nanoindentation Studies

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Advances in Polysaccharides: Practice & Applications

Novel Biocatalytic & Biopolymeric Approaches

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Recent Advances in Multiblock Copolymers

Synthesis

Sponsored by PMSE, Cosponsored by POLY‡

WEDNESDAY AFTERNOON

Section A

Moscone Center

120

General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

J. Su, Y. Teo, *Presiding*

1:00 POLY **534.** Synthesis and organocatalytic polymerization of azacaprolactones. **C. Turlington**, R.M. Waymouth

1:20 POLY **535.** Synthesis and self-assembly of brush block copolymers with various grafting densities. **T. Lin**, A. Chang, C. Bates, R.H. Grubbs

1:40 POLY **536.** Surprising and diverse reactivities of cyclopropenes in ring-opening metathesis polymerization. **J. Su**, Y. Xia

2:00 POLY **537.** Deprotonated ureas as simple, ultra-fast and highly selective super catalysts for ring-opening polymerizations. **B. Lin**

2:20 POLY **538.** Synthesis and characterization of crosslinked biodegradable polymers obtained using a redox-triggered crosslinking reaction. **K.R. Delle Chiaie**, A.B. Biernesser, L. Yablon, A.W. Sudyn, G.R. Michalowski, J.A. Byers

2:40 POLY **539.** Going beyond ruthenium in metal-cation-based anion exchange membranes. **M. Kwasny**, G.N. Tew

3:00 POLY **540.** Polyladders: A new polymer architecture via ROMP of rigid ladder motifs. **Y. Teo**, Y. Xia

3:20 POLY **541.** Prolines as efficient catalyst for stereocontrolled polymerization of rac-lactide. **H. Sardon**, A. Sanchez-sanchez, I. Rivilla, A. Basterrechea, M. Agirre, D. Mecerreyes, F. Cossio

3:40 POLY **542.** Taking charge of thiol-allylic ionic liquid photopolymerizations. **A. Tibbits**, L. Mumper, Y. Yan, C.J. Kloxin

4:00 POLY **543.** Silsesquioxane-based thermosetting phenylethynyls: Synthesis, thermally induced crosslinking and thermophysical properties. **T.S. Haddad**, G.R. Yandek, J. Zavala, J. Lamb, J. Reams, K. Ghiassi, J.M. Mabry, A.J. Guenthner

4:20 POLY **544.** New synthetic route to tetraarylphosphonium polyelectrolytes *via* Pd (0) catalyzed polycondensation from diols and diphenylphosphine. **W. Wan**, X. Yang, R. Smith

4:40 POLY **545.** Thioimidates: Fast and selective catalysts for ring-opening polymerizations. **X. Zhang**, R.M. Waymouth

Section B

Moscone Center

121

Next Generation Smart Materials

Cosponsored by MPPG‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

Y. Dong, B. L. Nichols, *Presiding*

1:00 Introductory Remarks.

1:05 POLY **546.** Enzyme-responsive nanoparticles for the targeted delivery of tetrazine-labeled proteins. **J. Michaelis**, P. Tufar, M.D. Burkart, N.C. Gianneschi

1:25 POLY **547.** Probing the causes of thermal hysteresis using tunable N_{agg} micelles with linear and brush-like thermoresponsive coronas. **L.D. Blackman**, M.I. Gibson, R.K. O'Reilly

1:45 POLY **548.** Mechanochemical fluorescence switching in polymers containing dithiomaleimide moieties. **M. Karman**, E. Verde-Sesto, Y.C. Simon, C. Weder

2:05 POLY **549.** Activation of a maleimide-anthracene mechanophore localized at a silica-polymer interface. **J. Sung**, M. Robb, J.S. Moore, S. White, N.R. Sottos

2:25 Intermission.

2:35 POLY **550.** CO_2/pH-responsive polymeric particles with built-in fluorescence read-out. **A.B. Mabire**, Q. Brouard, A. Pitto-Barry, R.J. Williams, H. Willcock, N. Kirby, E. Chapman, R.K. O'Reilly

2:55 POLY **551.** Preparing core-shell single molecules: Architecturally sound highly branched polymers with tuneable properties. **T. Swift**, R. Hoskins, S. Rimmer

3:15 POLY **552.** Optical devices constructed from responsive microgels for polyphenols detection. **S.M. Mugo**, M. Serpe, Q.M. Zhang

3:35 POLY **553.** Stimuli-Responsive helical dendronized polymers with switchable conformation. W. Li, K. Liu, **A. Zhang**

3:55 POLY **554.** Thermomechanical deformation of liquid crystalline elastomers: From flat to functional. **B.A. Kowalski**, C. Mostajeran, M. Warner, T.J. White

Section C

Moscone Center

122

Polymeric Materials for Performance & Sustainability

Recylable & Bio-Based Materials

Cosponsored by MPPG‡

M. Meador, M. A. Meador, S. E. Morgan, *Organizers*

J. Mates, *Presiding*

1:00 POLY **555.** Polymerizations with elemental sulfur: Sustainable fossil fuel chemistry. Y. Zhang, R.S. Glass, K. Char, **J. Pyun**

1:30 POLY **556.** Computational modeling of bio-based furan polymers and bio-inspired polymer adhesives. **I. Yeh**, C.B. Rinderspacher, J.J. La Scala, J.A. Orlicki, J. Lenhart, J. Andzelm

1:50 POLY **557.** Sugar-derived thermoresponsive block copolymers. **S. Wang**, J. He, M.B. Foston, T.H. Epps

2:10 POLY **558.** Oxidatively-cured coatings from renewable-based poly(vinyl ethers). **D. Kalita**, B.J. Chisholm, M.P. Sibi

2:30 Intermission.

2:45 POLY **559.** Effects of metal oxide loading on mechanical and rheological response in poly(vinylidene fluoride)-poly(lactic acid) composites. **J.M. McCollum**, J. Bencomo, S.T. Iacono

3:15 POLY **560.** Mechanistic investigation and kinetic modeling of PPV polymerization via Gilch using time-resolved low temperature and *in situ* UV-irradiation NMR-spectroscopy. **A. Schönbein**, M. Wagner, J. Kind, P.W. Blom, C.M. Thiele, J.J. Michels

3:35 POLY **561.** Incorporation of glucose in triblock copolymers to create sustainable adhesive and elastomeric materials. **M. Nasiri**, T.M. Reineke

3:55 POLY **562.** Chemorheology of a methacrylate based thermoplastic resin. **D. Cousins**, Y. Suzuki, J.R. Dorgan

Section D

Moscone Center

123

Polymers & Biomimicry

A. N. Dhinojwala, T. Williams, *Organizers*, *Presiding*

1:00 POLY **563.** Mimicking mussel adhesive proteins: How close can we get to the real thing? **J.J. Wilker**, S. Daily, N. Hamada, S.L. Huntington, T.A. Jones, M.G. Mazzotta, B. McGill, M. North, A. Putnam, H. Siebert, A. Tibabuzo

1:30 POLY **564.** Adhesion under humid conditions: Lessons from Spider Silk. **S. Singla**, G. Amarpuri, N. Dhopatkar, T.A. Blackledge, A.N. Dhinojwala

1:50 POLY **565.** Spiders tune glue viscoelasticity to maximize adhesion. **G. Amarpuri**, N. Dhopkatkar, T.A. Blackledge, A.N. Dhinojwala

2:10 POLY **566.** Solvent-Free, mussel-inspired polyester adhesives with impressive underwater adhesion. Y. Xu, A. Narayanan, Q. Liu, S. Kaur, A.N. Dhinojwala, **A. Joy**

2:40 Intermission.

‡ *Cooperative Cosponsorship*

2:55 POLY **567.** Paradigm shift in mussel-inspired adhesion. **K. Ahn**

3:25 POLY **568.** Poly(ester urea) based adhesives: Improved deployment and adhesion by incorporating poly(propylene glycol) segments. **V. Bhagat**, J. Zhou, M. Becker

3:45 POLY **569.** Constructing and deconstructing the barnacle adhesive interface. C.R. So, K.P. Fears, D. Barlow, D. Leary, C.M. Spillmann, **K.J. Wahl**

Section E

Moscone Center

124

Structure to Function in Supramolecular Polymers & Materials

R. Kieltyka, J. B. Matson, *Organizers*

P. Besenius, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 POLY **570.** Programmable brush polymer self-assembly via DNA hybridization. **K. Zhang**

1:30 POLY **571.** Self- and co-assemblies of BODIPY derivatives as drug nanocarriers. A. Rödle, A. Ramos Torres, V. Stepanenko, **G. Fernandez**

1:55 POLY **572.** Developing functional platforms for responsive materials and combination antimicrobials via non-covalent bonding in macromolecular systems. **J.C. Barnes**, A.F. Greene, X. Li

2:20 POLY **573.** Molecular organization, mechanical properties, and ion transport in hierarchically structured repeat-protein materials. **T. Zarkovic Grove**, N. Carter

2:45 POLY **574.** Active materials by coupling self assembly to the consumption of fuel. **R. Eelkema**, J. van Esch, G. Koper, J. Boekhoven, W. Hendriksen

3:10 Intermission.

3:25 POLY **575.** Super resolution imaging of supramolecular materials. **L. Albertazzi**

3:50 POLY **576.** Tunable structure and function of electrostatically self-assembled polymer nano-objects in solution. **F. Groehn**, A. Kutz, M. Wagner, A. Krieger, S. Frühbeißer, G. Mariani, R. Schweins

4:15 POLY **577.** Self-assembling Zwitterions as building blocks for switchable gels and polymers. **C. Schmuck**

4:40 POLY **578.** Reversible H- and J-type aggregation of a single perylene bisimide leading to different photoconductivity. **E. Draper**, M.A. Zwijnenburg, D.J. Adams

5:00 POLY **579.** Conductivity and mechanics in self-organized networks. **G.N. Tew**

Section F

Moscone Center

125

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Biomaterials

Cosponsored by PMSE

Financially supported by Wacker Chemical Corporation, Jewell Laboratories LLC

G. Wenz, *Organizer*

D. H. Thompson, *Organizer, Presiding*

I. Carneiro Leao, *Presiding*

1:00 POLY **580.** Structure-Activity relationships on the *in vivo* therapeutic efficacy of 2-hydroxypropyl-β-cyclodextrin:pluronic polyrotaxanes in Niemann-Pick type C disease. C.J. Collins, B. Loren, Y. Mondjinou, S. Alam, K. Haldar, **D.H. Thompson**

1:30 POLY **581.** Broad-spectrum anti-virals from cyclodextrins. **S. Jones**, F. Stellacci

2:00 POLY **582.** Withdrawn.

2:30 Intermission.

2:40 POLY **583.** Rapid enrichment of bacteria using a microfluidic device coupled with host-guest interactions. A. Pérez-Anes, A. Szarpak-Jankowska, D. Jary, G. Delapierre, **R. Auzely-Velty**

3:10 POLY **584.** Host-guest macromolecular assemblies: Interplay between macromolecular design, interactions and structure. **C. Amiel**, I. Antoniuk, B. Plazzotta, D. Kaczmarek, V. Wintgens, G. Volet, T. Nielsen, I. Varga, J. Pedersen

3:40 Intermission.

3:50 POLY **585.** Novel emulsions from palmitoyl cyclic sugar. **A. Cavac-Paulo**

4:20 POLY **586.** Self-assembly of responsive nanocontainers based on cyclodextrins. **B. Ravoo**

Section G

Moscone Center

Esplanade Ballroom 310

ACS Award in Polymer Chemistry: Symposium in honor of Murugappan Muthukumar

Cosponsored by PMSE

T. P. Lodge, *Organizer, Presiding*

V. M. Prabhu, *Presiding*

1:00 POLY **587.** Illumination alters the conformation and thermodynamics of conjugated polymers. B. Morgan, **M.D. Dadmun**

1:30 POLY **588.** Hierarchical structure and dynamics of oligocarbonate-functionalized PEG block copolymers. **V.M. Prabhu**

2:00 POLY **589.** Polymer physics to understand protein evolution under extreme temperature. **K. Ghosh**

2:30 POLY **590.** Rayleighian approach for studying the kinetics of ionic transport in polymeric media. **R. Kumar**

3:00 POLY **591.** Ohm's law, polymer electrolytes and lithium batteries. **N.P. Balsara**, D.M. Pesko

3:30 POLY **592.** Directing the phase behavior of polyelectrolyte complexes using chiral patterned peptides. N. Pacalin, L. Leon, **M.V. Tirrell**

4:00 POLY **593.** Effect of melt viscosity on self-nucleation of ethylene- and propylene-1-alkene random copolymers. **R.G. Alamo**

4:30 POLY **594. Award Address** (ACS Award in Polymer Chemistry sponsored by ExxonMobil Chemical Company). Polymer crystallization: New concepts and implications. **M. Muthukumar**

Bio-based Gels & Porous Materials

Biopolymer Organogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Polymers under Deformation

Control of Deformation across the Length Scale for Advanced Polymer Materials

Sponsored by PMSE, Cosponsored by MPPG‡ and POLY‡

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Advanced Materials & Structures

Sponsored by CELL, Cosponsored by MPPG‡ and POLY

Advances in Polysaccharides: Practice & Applications

Novel Materials & Methodologies

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Recent Advances in Multiblock Copolymers

Characterization

Sponsored by PMSE, Cosponsored by POLY‡

WEDNESDAY EVENING

Section A

Moscone Center

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POLY/PMSE Plenary Lecture & Awards

Cosponsored by PMSE

C. Lipscomb, C. R. Snyder, *Organizers*

C. L. Soles, *Presiding*

5:30 Welcome Reception.

6:45 POLY **595.** Directed assembly of hierarchical polymeric materials. **J.J. De Pablo**

7:30 Award Presentation and Reception.

THURSDAY MORNING

Section A

Moscone Center

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General Topics: New Synthesis & Characterization of Polymers

B. Barkakaty, D. Garcia, *Organizers*

A. E. London, N. Penfold, *Presiding*

8:00 POLY **596.** Chemical conversion of linkages in covalent organic frameworks. **P. Waller**, S.J. Lyle, T. Osborn Popp, C.S. Diercks, J.A. Reimer, O.M. Yaghi

8:20 POLY **597.** Effects of α-olefin chain length and monomer concentration on molecular weights and molecular weight distributions of various α-olefin-maleic anhydride copolymers. **H. Kim**, C. Tabasko, N.S. Khelfallah, J. Arroyave, R. Sharma

8:40 POLY **598.** Functional polyphosphoramidates and nanostructures with acid-triggered backbone cleavage. **H. Wang**, L. Su, R. Li, S. Zhang, K.L. Wooley

9:00 POLY **599.** Synthesis of bottlebrush polymers using the transfer-to approach. **S. Radzinski**, J. Foster, J. Matson

9:20 POLY **600.** Insight into the catalytic mechanism of metal-free ROMP – A DFT and experimental study. **J.C. Johnson**, T. Kensy, C.B. Rinderspacher, A.J. Boydston, D. Knorr

9:40 POLY **601.** Stimulus-responsive nonionic diblock copolymers: Protonation of a tertiary amine end-group induces vesicle-to-worm or vesicle-to-sphere transitions. **N. Penfold**, J. Lovett, P. Verstraete, J. Smets, S.P. Armes

10:00 POLY **602.** SI-RAFT Polymerization of chloroprene on silica nanoparticles for the application in rubber nanocomposites. **Z.M. Abbas**, Y. Zheng, M.M. Mohammadkhani, B.C. Benicewicz

10:20 POLY **603.** Hydrogen-bonded pore-switchable aqueous nanotubes via visible light-mediated room-temperature polymerization-induced self-assembly. P. Gao, Y. Ding, Z. Cui, **Y. Cai**

10:40 POLY **604.** Well-defined PDMAEA stars via Cu(0)-mediated reversible deactivation radical polymerisation. **R. Whitfield**, A. Anastasaki, N. Truong, P. Wilson, K. Kempe, T. Davis, D.M. Haddleton

11:00 POLY **605.** Hybrid nanoparticle-polymer brush composites for detection of radionuclides in water. **V. Bliznyuk**, A. Seliman, S.M. Husson, T.A. Devol

11:20 POLY **606.** pH-Responsive diblock copolymer nano-objects prepared by polymerization-induced self-assembly. **J. Lovett**, N. Warren, N. Penfold, C. Mable, S.P. Armes

Section B

Moscone Center

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Next Generation Smart Materials

Cosponsored by MPPG‡

E. B. Berda, J. Foster, Y. C. Simon, *Organizers*

Y. Dong, M. Karman, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **607.** Innovative bionanocomposites based on polysaccharides and protein nanofibers. **N.H. Silva**, I. Marrucho, C. Freire

8:25 POLY **608.** Withdrawn.

8:45 POLY **609.** Self-healing polymers for electronic skin, energy storage and actuators. **C. Wang**

9:05 POLY **610.** Synthesis of humidity-gradient responsive copolyamides via Retro-Michael reaction. **D.H. Wang**, R.N. McKenzie, P.R. Buskohl, R.A. Vaia, L. Tan

9:25 Intermission.

9:40 POLY **611.** Application of base amplification to extrinsic self-healing materials. **S. Lai**, T. Doan, W. Li, N.R. Sottos, P.V. Braun

10:00 POLY **612.** How to make a material predictive. **T. Raidt**, F. Katzenberg, J.C. Tiller

10:20 POLY **613.** Alkali-metal-ion accelerated on-demand release from cyclic poly(phthalaldehyde) microcapsules. **S. Tang**, H. Liu, J. Moore

10:40 POLY **614.** Shape memory polypropylene. **F. Katzenberg**, T. Raidt, J.C. Tiller

Section C

Moscone Center

122

Polymeric Materials for Performance & Sustainability

Applications

Cosponsored by MPPG‡

M. Meador, S. E. Morgan, *Organizers*

M. A. Meador, *Organizer, Presiding*

8:00 POLY **615.** Making wind power better – new polymer composites with improved sustainability metrics. **J.R. Dorgan**

8:30 POLY **616.** Hexagonal liquid crystal-carbon nanotube composites. **C.R. Kasprzak**, E. Scherzinger, J. Parkinson, S. Zhang

8:50 POLY **617.** Conjugated materials with multistage sidechains for water processable organic electronics. **B. Schmatz**, Z. Yuan, A. Lang, J. Hernandez, E. Reichmanis, J.R. Reynolds

9:10 POLY **618.** Driving performance in low VOC binder rich paints. **P.S. Majumdar**, D. Conner, P. Luo, S. Eberly, T.A. Phillips, P. Doll, G.W. Dombrowski

9:30 Intermission.

9:45 POLY **619.** Bio-based/biodegradable materials from thermoplastic cellulose and aliphatic polyester. **J.H. Wang**, B. Zhou

10:15 POLY **620.** Multifunctional materials based on nanofibers and open and closed cell aerogel foams for sustainability. **S.C. Jana**, N. Teo, S.J. Kim, S. Rajgarhia, M. Ghosh

10:45 POLY **621.** Robust porous polymers enabled by rapid TFA-etch with improved selectivity for polylactide. **A. Sarkar**, M. Stefik

Section D

Moscone Center

123

Polymers & Biomimicry

T. Williams, *Organizer*

A. N. Dhinojwala, *Organizer, Presiding*

8:00 POLY **622.** Making silk without silkworms: Using industrial biotechnology to make performance protein-based fibers. **D. Breslauer**

8:30 POLY **623.** Protein transduction domain mimics from simple polymer scaffolds. **G.N. Tew**

8:50 POLY **624.** Multi-compartmentalized polymersomes as structural analogues of eukaryotic cells. **A. Peyret**, E. Ibarboure, A. Tron, L. Beauté, R. Rust, O. Sandre, N. McClenaghan, S. Lecommandoux

9:10 POLY **625.** Understanding the effect of nanoparticle rigidity on the mechanism of cellular uptake. **P. Gurnani**, C. Sanchez Cano, S. Perrier

9:30 Intermission.

9:40 POLY **626.** Polypept(o)ides: Combining the functionality of polypeptides with the stealth-like properties of polysarcosine. **M. Barz**

10:00 POLY **627.** Synthetic antibodies. **A. Poma**, A. Guerreiro, H. Brahmbhatt, H. Pendergraff, J. Watts, G. Battaglia, N.W. Turner, S. Piletsky

10:20 POLY **628.** Permeable polymersomes as cascade nanoreactor protocells. **L.D. Blackman**, M.I. Gibson, R.K. O'Reilly

10:40 POLY **629.** Exploring principles of tissue morphogenesis and cancer progression using synthetic matrices. **X. Jia**

11:00 POLY **630.** Structural effects of relative side group locations on antibacterial and hemolytic activities of amphiphilic PEGylated macromolecules. **A. Punia**, E. He, K. Lee, N. Yang

11:20 POLY **631.** Generalized Manning model captures excess ion atmosphere around highly charged polymers. **U. Mohanty**

11:40 POLY **632.** Synthesis of a library of degradable and protein-stabilizing polyesters using thiol-ene post-polymerization modification. **E. Pelegri-O'Day**, S. Paluck, H.D. Maynard

Section E

Moscone Center

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Structure to Function in Supramolecular Polymers & Materials

P. Besenius, R. Kieltyka, J. B. Matson, *Organizers*

K. J. Arrington, B. Kemper, *Presiding*

8:00 Introductory Remarks.

8:05 POLY **633.** Recyclable elastomeric networks based on reversible cross-linking chemistry. **P. Berto**, F. Peruch, S. Grelier

8:25 POLY **634.** Topology transformable polymers derived by mechanical linkage. **T. Takata**

8:50 POLY **635.** Supramolecular structures of polymers around nanocarbons. **S. Zhang**

9:15 POLY **636.** Tensile property enhancement and photo-actuation of supramolecular self-assembled copolymers of P3HT. **T.M. Pathiranage**, J.M. Boothby, M.C. Biewer, T.H. Ware, M.C. Stefan

9:35 Intermission.

9:50 POLY **637.** Hydrogen bonding supramolecular polymers with temperature controlled switchable mechanical properties reveal photoheable effects. **A. Razgoniaev**, K. Mikhailov, F. Obrezkov, A. Ostrowski

10:10 POLY **638.** Regioselective, metal free C-C coupling of hexafluorobenzene for stable porous polymer networks. D. Thirion, V. Rozyyev, A. Adishev, **C.T. Yavuz**

10:35 POLY **639.** UV Patterned calixarene-derived supramolecular gels with spatially resolved mechanical and fluorescent properties. **J. Lee**, J.H. Jung, K. Sakurai

10:55 POLY **640.** Trefoil knotted block copolymer *via* ring-expansion strategy. **P. Cao**, L. Rong, J. Mangadlao, R.C. Advincula

11:15 POLY **641.** Perylene bisimide aggregation in water: Self-assembly features and development of stimuli responsive materials. **B. Soberats**, D. Görl, P. Syamala, F. Wuerthner

Section F

Moscone Center

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Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Stimuli-responsive Polymers & Polymer Processing

Cosponsored by PMSE

Financially supported by Wacker Chemical Corporation, Jewell Laboratories LLC

D. H. Thompson, G. Wenz, *Organizers*

A. Harada, K. Ito, *Presiding*

8:00 POLY **642.** Developing cyclodextrin-based 3D printing materials. Q. Lin, H. Wang, **C. Ke**

8:20 POLY **643.** Stimuli responsive nanoparticles from cyclodextrin polymers. **T. Nielsen**

8:40 POLY **644.** Preparation of shape memory polymers or self-healing composites based on cyclodextrin-based inclusion. Z. Chao, K. Guo, Y. Xiao, B. Li, **S. Zhang**

9:00 Intermission.

9:10 POLY **645.** Highly porous, mechanically strong, cyclodextrin-rich polyimide gels designed for advanced applications: Synthesis, characterization, and applications. **E. Leonhardt**, T. Williams, K.L. Wooley

9:30 POLY **646.** Monodisperse thermoresponsive cyclodextrins with switchable inclusion complexation. J. Yan, W. Li, K. Liu, **A. Zhang**

9:50 POLY **647.** Restructuring polymers *via* nano-confinement and subsequent release. **A.E. Tonelli**

10:20 Intermission.

10:30 POLY **648.** Controlled *rotaxa*-polymerization for well-defined polyrotaxanes. **G. Kali**, J. Hilschmann, G. Wenz

10:50 POLY **649.** Amphiphilic cyclodextrin functionalized surfaces. **K.L. Larsen**

11:10 POLY **650.** Polydiacetylenyl β-cyclodextrin based smart vesicles for colorimetric assay of arginine and lysine. E. Cho, H. Kim, Y. Choi, S. Paik, **S. Jung**

11:40 Concluding Remarks.

Bio-based Gels & Porous Materials

Aero-, Cryo- & Xerogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Commercial & Versatile Technology

Sponsored by CELL, Cosponsored by MPPG‡ and POLY

Advances in Polysaccharides: Practice & Applications

New Functional Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

Recent Advances in Multiblock Copolymers

Application

Sponsored by PMSE, Cosponsored by POLY‡

THURSDAY AFTERNOON

Bio-based Gels & Porous Materials

Open-Porous Carbon Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Reactive Extrusion: Advances at the Nexus of Polymer Processing, Materials Technology & Green Chemistry

Energy, Food & Packaging Development

Sponsored by CELL, Cosponsored by MPPG‡ and POLY

Advances in Polysaccharides: Practice & Applications

Preparation, Characterization & Applications

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Developments in the Fields of Celluloses & Lignocelluloses: In honor of Dr. Rajai Atalla

Sponsored by CELL, Cosponsored by AGFD, ANYL and POLY

‡ *Cooperative Cosponsorship*

PMSE

Division of Polymeric Materials Science and Engineering

A. Tsou, M. Grunlan, B. Olsen, X. Jia and C. Snyder, *Program Chairs*

OTHER SYMPOSIA OF INTEREST:

Advanced Materials & Technologies for Solar Energy Conversion & Storage (see *ENFL,* Sun, Mon, Tue)

Bio-based Gels & Porous Materials (see *CELL,* Wed, Thu)

Contributions of IBM Almaden to Polymer Science (see *POLY,* Sun, Mon)

Next Generation Smart Materials (see *POLY,* Sun, Mon, Tue, Wed, Thu)

Polymer Applications & Characterization in the Biomedical Industry (see *POLY,* Sun, Tue)

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications (see *POLY*, Tue, Wed, Thu)

SOCIAL EVENTS:

Reception, 5:30 PM: Wed

BUSINESS MEETINGS:

Executive Committee Meeting, 4:30 PM: Sun

Business Meeting, 5:00 PM: Mon

SUNDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 303

Young Investigator's Symposium

Cosponsored by DAC‡

Financially supported by Sigma-Aldrich, IBM, Solvay, Henkel, Tosoh, JACS, ACS Central Science, Chemistry of Materials, ACS Nano, Macromolecules, ACS Macro Letters, Chem (Cell Press)

L. Campos, J. M. Garcia, *Organizers*

W. Gutekunst, A. Obermyer, *Presiding*

9:00 PMSE **1.** Organic polymer chemistry in the context of novel processes. **J.M. Desimone**

9:30 PMSE **2.** Design of hydrogel-based synthetic extracellular matrix mimics for fundamental studies of disease and regeneration. **A.M. Kloxin**

10:00 PMSE **3.** Cartilage tissue engineering: Using soft material scaffolds. **G. O'Connell**

10:30 Intermission.

10:45 PMSE **4.** Piezo-chemical mediated ATRP via mechanical energy for self-improving materials. **A.P. Esser-Kahn**, H. Mohapatra, E. Sanders

11:15 PMSE **5.** Dynamic and user-programmable biomaterials for 4D cell culture. J.A. Shadish, L. Liu, **C.A. DeForest**

11:45 PMSE **6.** Better together: Biomanufacturing with microbial consortia. **M.A. O'Malley**

Section B

Moscone Center

Esplanade Ballroom 304

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Polymer Synthesis

Cosponsored by WCC

Financially supported by Chemistry of Materials (ACS Journal), Corning Inc., MilliporeSigma

Q. Lin, E. Reichmanis, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:40 PMSE **7.** Precisely functionalized molecular nanoparticles are unique elements for macromolecular science: From nanoatoms to giant molecules. **S.Z. Cheng**

9:10 PMSE **8.** Staging delivery nanomaterial approaches to address short and long term healing. **P.T. Hammond**

9:40 PMSE **9.** Vanishing polymers: Polymer systems designed to fail. **C.K. Ober**, A. Leonardi, K. Camera

10:10 Intermission.

10:30 PMSE **10.** Side chains in conjugated polymers: Designing beyond solubility. **J.R. Reynolds**

11:00 PMSE **11.** Polymeric semiconductor for high-performance field-effect transistor and circuit. **Y. Liu**

11:30 PMSE **12.** Synthesis, processing and function of coplanar π-conjugated organic polymers. **L. Fang**

Section C

Moscone Center

Esplanade Ballroom 305

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

R. Baumgartner, K. C. DeMella, *Presiding*

8:30 PMSE **13.** Functional polyesters for heat triggered norbornene thermosets. **R. Baumgartner**, K. Ryba, Z. Song, R. Wang, K. Harris, J.S. Katz, J. Cheng

8:50 PMSE **14.** Structured polymeric microparticles via aerosol cationic photopolymerization. **M. Bazzano**, R. Pisano, M. Woerner, S. Marco

9:10 PMSE **15.** Improving spin-cast epoxy telescope mirrors with spiro orthocarbonates, polyhedral oligomeric silsesquioxanes, and functionalized multi-walled carbon nanotubes. **K. Brodhacker**

9:30 PMSE **16.** Raman-active polymer dots for live cell imaging. **S. Brucks**, F. Hu, W. Min, L. Campos

9:50 PMSE **17.** Graphene as nanofiller: Tailoring the functionality for use in polymer nanocomposites. **L. Burk**

10:10 Intermission.

10:25 PMSE **18.** Polyisobutylene oligomers as tools for nanoparticle solubilization. **C. Chao**, P. Manyam, N. Riaz, R. Khanoyan, S. Madrahimov, D.E. Bergbreiter

10:45 PMSE **19.** Hybrid double network hydrogels with high strength and toughness. **H. Chen**, Q. Chen, F. Yang, K. Chu, R. Hu, M. Zhang, B. Ren, J. Zheng

11:05 PMSE **20.** Exploring the use of metalized nanocellulose in the supporting layer of polysulfone forward osmosis membranes: A water reclamation approach. **P.E. Cruz Tato**, L. Santiago-Martoral, K. Vega, E.O. Ortiz Quiles, E. Nicolau

11:25 PMSE **21.** Functionalized polymer foam sorbents for oil spill remediation. E. Barry, A. Mane, J. Libera, J. Elam, **S.B. Darling**

11:45 PMSE **22.** Photoresponsive multicompartment capsules for controlled release. **K.C. DeMella**, S.R. Raghavan

Section D

Moscone Center

Esplanade Ballroom 306

Janus Particles: Synthesis, Characterization & Applications

Cosponsored by COLL and MPPG‡

S. Bon, D. Lee, S. Sacanna, *Organizers*

E. Pentzer, *Organizer, Presiding*

D. Watkins, *Presiding*

9:00 PMSE **23.** Responsive Janus particles. **T.M. Swager**

9:30 PMSE **24.** Gram-scale synthesis of magnetic-semiconductor Janus nanoparticles: Ramifications for colloidal polymers. N.G. Pavlopoulos, N. Pinna, K. Char, **J. Pyun**

10:00 PMSE **25.** Fabrication and characterization of Golf-ball shaped microparticles based on the biodegradable polymers. **K. Cho**, S. Yoon, J. Yim

10:30 Intermission.

10:50 PMSE **26.** Synthesis of monodisperse bicompartmentalized amphiphilic Janus microparticles for tailored assembly at oil-water interface. **J. Kim**

11:20 PMSE **27.** Programmable self-assembly of 3-dimensional structures from micron-scale units. **B. Cassidy**, W. Glazener, K. Li, M. Li, C. Jung, A.D. Ellington, C.G. Willson

11:40 PMSE **28.** Shear-induced alignment of Janus particle lamellar structures. R.A. DeLaCruz-Araujo, D. Beltran-Villegas, R.G. Larson, **U.M. Cordova-Figueroa**

Section E

Moscone Center

Esplanade Ballroom 307

1D Nanomaterials: Synthesis, Assembly, Properties & Applications

Polymer-Based

S. B. Darling, J. Hahm, *Organizers*, *Presiding*

8:00 PMSE **29.** Gene regulation via co-assembled, noncationic DNA-polymer conjugates. **D. Wang**, F. Jia, X. Lu, X. Cao, X. Tan, K. Zhang

8:20 PMSE **30.** Nanostructured films for therapeutic delivery and wound healing. **T. Desai**

8:50 PMSE **31.** Optically active protein films inspired by cephalopods. **E. Leung**, L. Phan, A.A. Gorodetsky

9:10 PMSE **32.** Tetrazine mediated drug delivery. **J. Geng**, K. Neumann, S. Jain, M. Bradley

9:30 PMSE **33.** Investigating the dynamics of self-assembling cyclic peptide-polymer nanotubes. **J.Y. Rho**, J. Brendel, S. Perrier

9:50 Intermission.

10:05 PMSE **34.** Functional nanofibrous materials: Controllable fabrication and applications. **B. Ding**

10:25 PMSE **35.** Microwave structured polyamide-6 nanofiber/net membrane embedded with poly(m-phenylene isophthalamide) staple fibers for ultrafine particle filtration. **H. Liu**, S. Zhang, L. Liu, J. Yu, B. Ding

10:45 PMSE **36.** Bio-inspired nano-structured polymer thin films via self-assembly of magnetic nanoparticles. **A. Karim**, I.J. Zvonkina

11:05 PMSE **37.** Preparation and characterization of antimicrobial fibrous membranes based on polyhydroxybutyrate. **X. Ren**, X. Fan, T. Huang

11:25 PMSE **38.** Tunable peptide constructs for systematically controlling the structure and assembly of chiral gold nanoparticle single helices. **S. Mokashi Punekar**, A. Merg, N.L. Rosi

Section F

Moscone Center

Esplanade Ballroom 308

Nanoscale Spectroscopic Characterization of Catalysts & Polymers

NMR-Based Methods

Financially supported by Anasys Instruments, Bruker BioSpin, Bruker Nano, ExxonMobil Chemical Company, Neaspec

D. Yablon, *Organizer*

J. Rapp, *Organizer, Presiding*

8:30 PMSE **39.** Atomic-scale characterization of catalytic materials by advanced solid-state NMR methods. T. Kobayashi, F.A. Perras, **M. Pruski**

9:00 PMSE **40.** Understanding nanoscopic interfaces in tapered copolymers and their impact on macroscopic properties. **J.L. White**, A. Clough, J. Kelsey, J.J. Zhou

9:30 PMSE **41.** Model, fumed silica-supported catalysts: Characterization and performance. **M. Afeworki**, P. Brant

10:00 Intermission.

10:10 PMSE **42.** Solid-state NMR characterization of rare-earth nanoparticles. D.A. Hirsh, B. Richard, N. Johnson, A. Ritcey, F. Van Veggel, **R.W. Schurko**

10:40 PMSE **43.** Early time kinetics and mechanisms of polymerization reactions by hyperpolarized NMR. C. Chen, W. Shih, **C. Hilty**

11:10 PMSE **44.** Structure and dynamics at interfaces in hybrid materials. **U. Scheler**

Section G

Moscone Center

Esplanade Ballroom 309

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

M. J. Derry, L. E. Hanzly, *Presiding*

8:30 PMSE **45.** Shear-induced alignment of diblock copolymer worm gels. **M.J. Derry**, O. Mykhaylyk, S.P. Armes

8:50 PMSE **46.** Combining spray and atmospheric plasma deposition of transparent bilayer protective coatings on plastics for exceptional adhesion and hardness. **Y. Ding**, S. Dong, D. He, Z. Zhao, R. Dauskardt

9:10 PMSE **47.** Withdrawn.

9:30 PMSE **48.** Dual precursor atmospheric plasma deposition of organosilicate transparent functional coating on plastics. **S. Dong**, Y. Ding, D. He, Z. Zhao, R. Dauskardt

9:50 PMSE **49.** Manipulating ordering and alignment in nanostructured thin films by combining substrate and solvent annealing effects. **T.H. Epps**, C.K. Shelton

10:10 Intermission.

10:25 PMSE **50.** Harnessing the interaction between surfactant and catalyst to control ATRP in dispersed media. **M. Fantin**, Y. Wang, P. Chmielarz, F. Lorandi, **K. Matyjaszewski**

10:45 PMSE **51.** Metal coordination complexes in mechanically responsive systems. **K. Hall**, M.H. Horst, S.W. Telford, K.J. Franz

11:05 PMSE **52.** Helical lipopeptide with enhanced antimicrobial activity. **Z. Han**, M. Xiong, J. Cheng

11:25 PMSE **53.** Protein self-assembly in polar polymer environments of varying viscosity. **L.E. Hanzly**, J.R. Barone

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Separation of Macromolecules & Particulates

Sponsored by POLY, Cosponsored by ANYL, COLL and PMSE

Incorporating Polymer Science into the Classroom

Undergraduate Curriculum

Sponsored by POLY, Cosponsored by CHED, MPPG‡ and PMSE

Contributions of IBM Almaden to Polymer Science

Sponsored by POLY, Cosponsored by PMSE

SUNDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 303

Young Investigator's Symposium

Cosponsored by DAC‡

Financially supported by Sigma-Aldrich, IBM, Solvay, Henkel, Tosoh, JACS, ACS Central Science, Chemistry of Materials, ACS Nano, Macromolecules, ACS Macro Letters, Chem (Cell Press)

L. Campos, J. M. Garcia, *Organizers*

V. Piunova, J. Qin, *Presiding*

1:30 PMSE **54.** Doing more with controlled radical polymerization. **C.J. Hawker**

2:00 PMSE **55.** Polymeric nanomaterials for tailoring the functions of the cellular glycocalyx. **K. Godula**

2:30 PMSE **56.** Shaping the future of polymer molecular weight distributions. **B.P. Fors**

3:00 PMSE **57.** Rational synthesis of semiconductor fragments. **R.S. Klausen**

3:30 Intermission.

3:45 PMSE **58.** Design and development of negative photochromic systems. **J. Read De Alaniz**

4:15 PMSE **59.** Orthogonally responsive small molecule dyes in polymer films: Data storage in 0, 1, 2, 3. P. Wei, B. Li, A.C. de Leon, **E. Pentzer**

4:45 PMSE **60.** Ultrafast gelation of injectable reactive microgels: The power of TAD click chemistry. R. Absil, S. Çakir, R. Teixeira, G. Rivero, S. Gabriele, P. Dubois, C. Barner-Kowollik, F.E. Du Prez, **L.M. Mespouille**

Section B

Moscone Center

Esplanade Ballroom 304

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Advances in Organic Solar Cells

Cosponsored by WCC

Financially supported by Chemistry of Materials (ACS Journal), Corning Inc., MilliporeSigma

Q. Lin, E. Reichmanis, *Organizers*, *Presiding*

1:30 PMSE **61.** New polymers and synthetic strategies to polymers for photovoltaic and perovskite solar cells. **A. Facchetti**

2:00 PMSE **62.** Development of organic semiconducting polymers: Toward real applications. **M. He**, W. Niu, J.R. Matthews, A. Wallace

2:30 PMSE **63.** Benzotriazole: A versatile building block for conjugated polymers based solar cells. **W. You**

3:00 Intermission.

3:30 PMSE **64.** Ternary organic solar cells. **T.P. Russell**

4:00 PMSE **65.** Melt-processable complementary semiconducting polymer blends for organic electronics. **J. Mei**

4:30 PMSE **66.** Graphene-polymer and nanocarbon-polymer composites for cellular mechanics and wireless, wearable sensors. **D.J. Lipomi**

5:00 PMSE **67.** Single crystal Rubrene: Tested and proven. **A.L. Briseno**

Section C

Moscone Center

Esplanade Ballroom 305

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

J. N. Lo, K. P. Mineart, *Presiding*

1:30 PMSE **68.** Post-printing functionalization of radiopaque amino acid based poly(ester urea)s. **S. Li**, Y. Xu, M. Becker

1:50 PMSE **69.** CO_2-responsive poly(N,N-dimethylaminoethyl methacrylate) hydrogels with fast responsive rate. **X. Li**, R. Xie, Z. Jia, X. Ju, W. Wang, Z. Liu, L. Chu

2:10 PMSE **70.** Eliminating porosity in benzoxazine thermosets. **J.N. Lo**, X. Zhang, T.J. Williams, S. Nutt

2:30 PMSE **71.** Elettrochemically mediated ATRP on non-Pt electrodes, in organic and aqueous media. **F. Lorandi**, M. Fantin, A. Amhed Isse, A. Gennaro

2:50 PMSE **72.** Thiol-ene networks for triplet-triplet annihilation. **J. Lott**, A. Jentsch, B. Davis

3:10 Intermission.

3:25 PMSE **73.** Chiral self-assembly of achiral π-conjugated polyelectrolytes induced by hyaluronic acid. **P. Manandhar**, T. Vokata, J. Moon

3:45 PMSE **74.** Solvent stable electrospun membranes developed through ultraviolet induced reactive electrospinning. **M.F. Mehmood**, N.P. Gule, S. Marco, P. Mallon

4:05 PMSE **75.** Novel surface grafting chemistries for the functionality manipulation of composite separation membranes. **J. Meng**

4:25 PMSE **76.** Hybrid stealth liposomes via incorporation of cholesterol-functionalized diblock copolymers. **K.P. Mineart**, S. Venkataraman, Y. Yang, J. Hedrick, V. Prabhu

4:45 PMSE **77.** Enhancement of sulfonated polyphenelyne properties as a proton conducting membrane by blending with novel polysulfone-base polymer. **B. Motealleh**, T.D. Largier, C.J. Cornelius

Section D

Moscone Center

Esplanade Ballroom 306

Janus Particles: Synthesis, Characterization & Applications

Cosponsored by COLL and MPPG‡

S. Bon, E. Pentzer, S. Sacanna, *Organizers*

D. Lee, *Organizer, Presiding*

L. Bradley, *Presiding*

1:30 PMSE **78.** External-field induced propulsion of particles with broken symmetry. **N. Wu**

2:00 PMSE **79.** UV-triggered decoration of Janus micro/nano particles. **N. Razza**, S. Marco

2:20 PMSE **80.** Controlling morphology and nanoparticle location within hybrid polymer-inorganic Janus particles using flash nanoprecipitation. **V. Lee**, C. Sosa, R. Liu, R.K. Prudhomme, R.D. Priestley

2:40 PMSE **81.** Propoulsion of metallodielectric Janus particles by contact charge electrophoresis. **K. Bishop**, Y. Dou, C. Cartier, W. Fei, S. Pandey, S. Razavi, I. Kretzschmar

3:10 Intermission.

3:30 PMSE **82.** Self-assembly and reconfiguration of Janus ellipsoids at high concentrations. **M.J. Solomon**, S. Razavi, Y. Liu

4:00 PMSE **83.** Synthesis of highly tailorable nanoparticle combinatorial libraries. **J. Hedrick**, P. Chen, E.J. Kluender, B. Meckes, C.A. Mirkin

4:20 PMSE **84.** Synthesis, self-assembly and collective behaviors of asymmetric motile rodlike colloids. Y. Yang, A. Gyedu, K. Liu, **Z. Nie**

Section E

Moscone Center

Esplanade Ballroom 307

1D Nanomaterials: Synthesis, Assembly, Properties & Applications

Polymer-Based

S. B. Darling, J. Hahm, *Organizers*, *Presiding*

1:00 PMSE **85.** PVA silica composite nanofibers via sol gel electrospinning. **T. Pirzada**, S. Arvidson, C.D. Saquing, S. Shah, S.A. Khan

1:20 PMSE **86.** Mesoporous block copolymer nanofibers by selective swelling. X. Shi, **Y. Wang**

1:50 PMSE **87.** Electrospun nanofibrous materials for CO_2 capture. **X. Wang**, B. Ding, J. Yu

2:10 PMSE **88.** Electrospun nanofiber composite as proton exchange membrane for fuel cell. **B. Motealleh**, F. Huang, T.D. Largier, C.J. Cornelius

2:30 PMSE **89.** Programming the orientation of carbon nanotubes in liquid crystalline elastomers. **T. Guin**, A.D. Auguste, B. Kowalski, V. Tondiglia, T.J. White

2:50 Intermission.

3:05 PMSE **90.** Development and studies of DBfA/DfA block copolymers for optoelectronics. **S.S. Sun**, M. Hasib, T.H. Nguyen

3:25 PMSE **91.** Enticing and general strategy for 1D nanocrystals with unprecedented control over dimensions, compositions and architectures using bottlebrush-like block copolymers as nanoreactors. **Z. Lin**

3:55 PMSE **92.** Multilevel structured polysulfone/polyacrylonitrile/polyamide-6 nanofiber/nets membranes for sieving airborne particles. **N. Tang**, S. Zhang, J. Yu, B. Ding

4:15 PMSE **93.** Molecular design of poly(3-hexylthiophene)-graft-poly(2-vinylpyridine) copolymers to control the crystallinity for solution-assembled nanowires. **Y. Kim**, H. Kim, J. Kim, R.C. Hayward, B. Kim

5 dendronized polymers with increased structural perfection: Approaching g_{max} of cylindrical nano-objects. **D. Messmer**, D. Schlueter

‡ *Cooperative Cosponsorship*

Section F

Moscone Center

Esplanade Ballroom 308

Nanoscale Spectroscopic Characterization of Catalysts & Polymers

Raman & SFG

Financially supported by Anasys Instruments, Bruker BioSpin, Bruker Nano, ExxonMobil Chemical Company, Neaspec

J. Rapp, D. Yablon, *Organizers*

Z. Su, *Presiding*

1:30 PMSE **95.** Confocal Raman microscopy of the in-situ uniaxial deformation of a polyethylene dog bone. C.R. Lopez-Barron, Y. Zeng, **J. Schaefer**, A. Eberle, T.P. Lodge, F.S. Bates

2:00 PMSE **96.** Scanning angle Raman spectroscopy measurements of thin polymer films and buried polymer interfaces. **E.A. Smith**, J.M. Bobbitt, D. Mendivelso-Perez, C. Nyamekye

2:20 Intermission.

2:30 PMSE **97.** Predicting Raman spectra of condensed polymer phases from simulations. **Q. Chen**, S. Milner

2:50 PMSE **98.** Spatially resolved EDS and Raman characterization of crosslinked polymeric catalysts biomass hydrolysis. M.V. Tyufekchiev, P. Duan, M.T. Timko, M. Emmert, K. Schmidt-Rohr, **S. Granados Focil**

3:10 PMSE **99.** Effect of interfacial molecular orientation on power conversion efficiency of perovskite solar cell. **M. Xiao**, J. Jasensky, Z. Chen

Section G

Moscone Center

Esplanade Ballroom 309

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

J. A. Nikles, K. Olson, *Presiding*

1:30 PMSE **100.** Genetically encoded lipid-polypeptide hybrid biomaterials. **D. Mozhdehi**, K.M. Luginbuhl, J. Simon, M. Dzuricky, F. Huang, K.L. Buehne, N.R. Mayne, A. Chilkoti

1:50 PMSE **101.** Withdrawn.

2:10 PMSE **102.** High performance multistage-stage cure resins for Continuous Liquid Interface Production (CLIP). **A. Nebipasagil**, A.L. Quintanilla, S.J. Mecham, J. Cushen, J. Rolland, J.M. DeSimone

2:30 PMSE **103.** Kinetics of drug release from polymer micelles. **J.A. Nikles**, L.N. Cobb, J.A. Gettinger, B.J. McCormick, S.M. Nikles, A.L. Glover, C.S. Brazel, D.E. Nikles

2:50 Intermission.

3:05 PMSE **104.** Chitosans in nanostructured films for biosensing and antimicrobial coatings. **O.N. Oliveira**

3:25 PMSE **105.** Developing nonflammable perfluoropolyether electrolytes for safe lithium-ion batteries. **K. Olson**, M. Chintapalli, K. Timachova, J. Yin, A.C. Marschilok, E.S. Takeuchi, K.J. Takeuchi, S.J. Mecham, N.P. Balsara, J.M. Desimone

3:45 PMSE **106.** Recruiting physisorbed water for green and bio-degradable perfluorinated surface modifications. **S. Oyola-Reynoso**, J. Chen, B. Chang, J. Bloch, M. Thuo

4:05 PMSE **107.** Fluorescent block copolymer-MoS_2 nanohybrids for real-time photothermal heating and imaging. **C. Park**, B. Kim

4:25 PMSE **108.** Functional nanogels for decoration of biointerfaces. **A. Pich**, A. Töpel

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Separation of Macromolecules & Particulates

Sponsored by POLY, Cosponsored by ANYL, COLL and PMSE

Incorporating Polymer Science into the Classroom

High School & Community College

Sponsored by POLY, Cosponsored by CHED, MPPG‡ and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage

Cathode Materials

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Contributions of IBM Almaden to Polymer Science

Sponsored by POLY, Cosponsored by PMSE

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Homogeneous Catalysis

Sponsored by INOR, Cosponsored by PMSE

MONDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 303

Young Investigator's Symposium

Cosponsored by DAC‡

Financially supported by Sigma-Aldrich, IBM, Solvay, Henkel, Tosoh, JACS, ACS Central Science, Chemistry of Materials, ACS Nano, Macromolecules, ACS Macro Letters, Chem (Cell Press)

L. Campos, J. M. Garcia, *Organizers*

J. Kalow, K. Mirica, *Presiding*

9:00 PMSE **109.** Cancer immune therapy targeting the cell surface glycocalyx. **C.R. Bertozzi**

9:30 PMSE **110.** Functional ladder materials enabled by efficient catalysis. **Y. Xia**

10:00 PMSE **111.** Synthesis of polythioaminals using in-situ generated imines as reactive intermediates: Polymers for tailorable surface topology. **R. Wojtecki**

10:30 Intermission.

10:45 PMSE **112.** Convergence of high rate and selectivity in organocatalytic ring-opening polymerization. **M.K. Kiesewetter**, E. Kiesewetter, K. Fastnacht, S. Spink

11:15 PMSE **113.** Block copolymers and crosslinked copolymers obtained with redox-switchable polymerization catalysts. **J.A. Byers**, K.R. Delle Chiaie, A.B. Biernesser, A.W. Sudyn

11:45 PMSE **114.** Generation, stability and applications of gelified foams. **C. Monteux**, F. Lequeux, R. Deleurence, T. Saison

Section B

Moscone Center

Esplanade Ballroom 304

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Novel Organic Materials

Cosponsored by WCC

Financially supported by Chemistry of Materials (ACS Journal), Corning Inc., MilliporeSigma

Q. Lin, E. Reichmanis, *Organizers*, *Presiding*

8:30 PMSE **115.** Enhanced ionic conductivity of peg-containing polyimide/ionic liquid membrane upon thermal annealing. **C.W. Frank**, E.T. Woo, J. Lu, E. Coletta, J. Mun, A. Spakowitz, D.Y. Yoon, M. Toney

9:00 PMSE **116.** Supramolecular free radicals. **X. Zhang**

9:30 PMSE **117.** Designing functional interfaces using click chemistry. **J.J. Locklin**

10:00 Intermission.

10:30 PMSE **118.** Super-wettability based fabrication of organic functional materials. **L. Jiang**

11:00 PMSE **119.** Nanostructured polymer gels as a multifunctional material platform for energy and responsive electronics. **G. Yu**

11:30 PMSE **120.** Alternative architectures and polymer coupling layers for field-effect biosensors. **H.E. Katz**

Section C

Moscone Center

Esplanade Ballroom 305

Support & Activator Effects on Metal Mediated Polymerization

Cosponsored by CATL, INOR and MPPG‡

Financially supported by ExxonMobil Chemical Company, Argonne National Laboratory

M. Delferro, *Organizer*

L. Luo, *Organizer, Presiding*

J. Severn, *Presiding*

8:00 PMSE **121.** Methylaluminoxane as activator for olefin polymerization catalysts. **W. Kaminsky**

8:25 PMSE **122.** Unexpected activation modes of constrained geometry precatalysts. **J. Klosin**

8:50 PMSE **123.** Structure, function, and modelling of MAO catalyst activators. **M. Bochmann**, F. Ghiotto, D. Rosca, M. Linnolahti

9:15 PMSE **124.** Actively supporting the world's strongest fiber. **J. Severn**

9:40 Intermission.

10:00 PMSE **125.** Effect of formation of ionic aggregates higher than ion pairs on the kinetics of a single olefin insertion into the Zr-C bond. **C. Zuccaccia**, A. Macchioni, L. Sian

10:25 PMSE **126.** Evidence of coordinated Trimethylaluminum (TMA) in Methylaluminoxane (MAO) as the major active site and its quantification. **L. Luo**, A. Jain, J. Harlan

10:50 PMSE **127.** Late transition metal sites supported on sulfated oxides for polymerization reactions. **M.P. Conley**

11:15 PMSE **128.** Surface-supported and solution phase homoleptic rare earth silazido catalysts. **A.D. Sadow**

Section D

Moscone Center

Esplanade Ballroom 306

Janus Particles: Synthesis, Characterization & Applications

Cosponsored by COLL and MPPG‡

S. Bon, D. Lee, E. Pentzer, *Organizers*

S. Sacanna, *Organizer, Presiding*

9:00 PMSE **129.** Seeded emulsion polymerization for non-spherical particles and clickable Janus colloids. **L. Bradley**, W. Chen, F. Tu, K.J. Stebe, D. Lee

9:30 PMSE **130.** Janus graphene oxide: Preparation and characterization. **A.C. de Leon**

9:50 PMSE **131.** Seeing the unseen: Interrogating intracellular dynamics using Janus particles. **Y. Yu**

10:20 Intermission.

10:40 PMSE **132.** Transport of active Janus particles in geometrically-confined spaces. **D. Velegol**, A. Sen, S. Das, A. Garg

11:10 PMSE **133.** Synthesis and characterization of janus linear-dendrtic hybrids as next generation biomateials. **D.G. Abebe**, D.L. Watkins

11:30 PMSE **134.** Synthesis and assembly of mono-patch particles. **G. Yi**, S. Kim, D. Pine, S. Sacanna, J. Oh

Section E

Moscone Center

Esplanade Ballroom 307

Synthesis, Processing & Device Engineering of Polymeric Electronic Materials

Financially supported by Tosoh, Japan Analytical Industry (JAI) Co., Ltd

L. Fang, J. Mei, *Organizers*

C. Di, *Organizer, Presiding*

8:00 PMSE **135.** Polymer molecular design and processing for efficient macroscale charge transport pathways. **E. Reichmanis**

8:30 PMSE **136.** Melt-processable complementary semiconducting polymer blends for organic field-effect transistors. **Y. Zhao**, X. Zhao, A. Gumyusenge, J. Mei

8:45 PMSE **137.** Degradable and biocompatible conjugated polymer for solution-processed imperceptible transient electronics. **T. Lei**, Z. Bao

9:05 PMSE **138.** Design and synthesis of semiconducting polymers for high-performance field-effect transistors. **Y. Liu**

9:35 PMSE **139.** Room-temperature air-stable spin transport in molecular-based multipurpose spin valves. **X. Sun**

9:55 Intermission.

10:15 PMSE **140.** Traps in conjugated polymers: Morphological and disorder effects. **A. Salleo**

10:45 PMSE **141.** Thioxanthone derivatives and their application for OLEDs. **Y. Wang**

11:05 PMSE **142.** Deep-blue light-emitting polymers containing spiro[fluorene-9,9′-thioxanthene-S,S-dioxide] isomers. F. Peng, **W. Yang**, Y. Cao

11:25 PMSE **143.** Making light with light: Patterning LED pixels from solution. **Z.A. Page**, B. Narupai, C. Pester, D.S. Laitar, A. Sokolov, S. Mukhopadhyay, R. Bou Zerdan, A. McGrath, K. Kearns, J. Kramer, C.J. Hawker

Section F

Moscone Center

Esplanade Ballroom 308

Nanoscale Spectroscopic Characterization of Catalysts & Polymers

Infrared-Spectroscopy-Based Methods

Financially supported by Anasys Instruments, Bruker BioSpin, Bruker Nano, ExxonMobil Chemical Company, Neaspec

J. Rapp, *Organizer*

D. Yablon, *Organizer, Presiding*

9:00 PMSE **144.** Measuring correlated chemical composition and thermal conductivity at the nanoscale with AFM probes. **A. Centrone**

9:30 PMSE **145.** Investigation of nanodomain composition in high-impact polypropylene by AFM-IR. **P. Bao**, Z. Su, F. Tang

10:00 Intermission.

10:10 PMSE **146.** How do biofilms eat their food? Understanding microbiological degradation of polyurethanes at the nanoscale with AFM-IR. **D. Barlow**, J.C. Biffinger, C. Hung, L.J. Nadeau, T. Zicht, A.L. Crouch, J.N. Russell, W.J. Crookes-Goodson

10:40 PMSE **147.** Nanoscale infrared spectroscopy for the chemical characterization of polymer systems. **E. Dillon**, C. Prater, K. Kjoller

11:00 PMSE **148.** Nano-FTIR: Quantitative infrared imaging and spectroscopy at 10nm spatial resolution. **A.J. Huber**

Section G

Moscone Center

Esplanade Ballroom 309

Molecular Engineering of Peptide Assembly

Protein Assembly

Financially supported by ACS Biomacromolecules

A. Kros, S. L. Perry, *Organizers*

H. Cui, M. V. Tirrell, *Organizers*, *Presiding*

8:10 Introductory Remarks.

8:15 PMSE **149.** Self-assembled fibrils composed of protein-based polymers with silk-like domains: Multiple roles for hydrophilic side-chains. L. Beun, S. Dhayal, L. Albertazzi, M. Werten, F. de Wolf, M.C. Stuart, **R. de Vries**

8:45 PMSE **150.** Self-assembly of stimulus responsive biohybrid polymers. **A. Chilkoti**

9:15 PMSE **151.** Self-assembled protein-inorganic hybrid supraparticles for enzyme immobilization. W. Park, A. Caparco, **J. Champion**

9:45 Intermission.

10:00 PMSE **152.** Minimal DNA length needed for the assembly of virus coat proteins. S. Maassen, M. de Ruiter, **J.J. Cornelissen**

10:30 PMSE **153.** Environmental influence on assembly landscapes in protein materials. C. Chen, J. Tan, M. Hsieh, A. Rha, R. Rengifo, J. Goodwin, A. Mehta, N. Anthony, M. Grover, **D.G. Lynn**

11:00 PMSE **154.** Electrostatic effects on self-assembly in protein-polymer block copolymers. **B.D. Olsen**, D. Chang, C. Lam, C. Mills

11:30 PMSE **155.** Design of polypeptide and protein-based copolymer self-assembled biomaterials. **S. Lecommandoux**, E. Garanger

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage

Flow Batteries & Organic Electrodes

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

50th Anniversary Celebration of Macromolecules

Sponsored by POLY, Cosponsored by MPPG‡ and PMSE

Contributions of IBM Almaden to Polymer Science

Sponsored by POLY, Cosponsored by PMSE

MONDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 303

Young Investigator's Symposium

Cosponsored by DAC‡

Financially supported by Sigma-Aldrich, IBM, Solvay, Henkel, Tosoh, JACS, ACS Central Science, Chemistry of Materials, ACS Nano, Macromolecules, ACS Macro Letters, Chem (Cell Press)

L. Campos, J. M. Garcia, *Organizers*

E. A. Appel, S. A. Sydlik, *Presiding*

1:30 PMSE **156.** Magnetically-active hybrid inorganic-organic network materials. J.A. Flores, A. Jahnke, A. Pavia Sanders, **K.L. Wooley**

2:00 PMSE **157.** Molecular precision and enzymatic disassembly of polymeric micelles. A.J. Harnoy, M. Segal, M. Buzhor, G. Slor, I. Rosenbaum, **R.J. Amir**

2:30 PMSE **158.** Controlled synthesis of π-conjugated polymers. **D.S. Seferos**

3:00 PMSE **159.** Influence of conjugated polymer thin-film morphology and exciton-plasmon coupling on nanophotonic light trapping and light extraction. **D. O'Carroll**

3:30 Intermission.

3:45 PMSE **160.** Functional organic frameworks in solution and thin films. **Y. Liu**, H. Wang, S. Cai, B. He, Z. Li, J. Tian, D. Zhang

4:15 PMSE **161.** Elastomeric and fluidic metamaterials: Towards large-area, reconfigurable metamaterials. **J. Dionne**

4:45 PMSE **162.** Structural engineering of sp^2 functional polymer materials at the molecular and nanoscopic scales. **L. Fang**

Section B

Moscone Center

Esplanade Ballroom 304

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Frontiers in Organic & Flexible Electronics

Cosponsored by WCC

Financially supported by Chemistry of Materials (ACS Journal), Corning Inc., MilliporeSigma

Q. Lin, E. Reichmanis, *Organizers*, *Presiding*

1:30 PMSE **163.** How do we design organic and inorganic materials for flexible, transparent electronic circuitry? **T.J. Marks**

2:00 PMSE **164.** Design and applications of dopants and acceptors for organic electronic applications. **S.R. Marder**

2:30 PMSE **165.** Advances in fabrication: A discussion. **J.M. Desimone**

3:00 Intermission.

3:30 PMSE **166.** Development of new electron acceptors for high efficient, non-fullerene OPV solar cells. **L. Yu**

4:00 PMSE **167.** Approaches to sustainable materials and processes for flexible electronics. G. Zhang, B. Risteen, P. Chu, **E. Reichmanis**

4:30 PMSE **168. Award Address** (ACS Award in Applied Polymer Science sponsored by Eastman Chemical Company). Skin-inspired polymer electronic materials. **Z. Bao**

Section C

Moscone Center

Esplanade Ballroom 305

Support & Activator Effects on Metal Mediated Polymerization

Cosponsored by CATL, INOR and MPPG‡

Financially supported by ExxonMobil Chemical Company, Argonne National Laboratory

M. Delferro, L. Luo, *Organizers*

R. L. Kuhlman, S. L. Scott, *Presiding*

1:00 PMSE **169.** Single site catalysis: How to avoid co-catalysts in polymerization. **J.M. Basset**, J. Pelletier

1:25 PMSE **170.** Withdrawn.

1:50 PMSE **171.** Activator effects in ATRP. **K. Matyjaszewski**

2:15 PMSE **172.** Impact of silica structure on the distribution of activator on supported catalyst particles. **X. Ye**

2:40 Intermission.

3:00 PMSE **173.** C–H activation and olefin insertion of $Cp^{Alkyl}Hf(IV)$-complexes observed by NMR and mass spec during olefin polymerization. **R.L. Kuhlman**, A. Gies, L. Tensi, C. Zuccaccia, A. Macchioni

3:25 PMSE **174.** Keltan ACE™ technology: Activation of post-metallocene EPDM polymerization catalysts. **G. van Doremaele**, M. Valla, R. Bernardo, A. Berthoud

3:50 PMSE **175.** Group 4 complexes in the homopolymerization and copolymerization of olefins. **M.S. Eisen**

4:15 PMSE **176.** New insights into activating metallocene catalysts for olefin polymerization. **C.G. Blakley**, M.G. Thorn, S.P. Diefenbach

Section D

Moscone Center

Esplanade Ballroom 306

Janus Particles: Synthesis, Characterization & Applications

Cosponsored by COLL and MPPG‡

D. Lee, E. Pentzer, S. Sacanna, *Organizers*

S. Bon, *Organizer, Presiding*

A. V. Zhukhovitskiy, *Presiding*

1:30 PMSE **177.** Design and assembly of asymmetrically functionalized particles via digital alchemy. **S.C. Glotzer**, G. Van Anders

2:00 PMSE **178.** Catalytic propulsion and magnetic steering of soft, patchy microcapsules: Ability to pick-up and drop-off microscale cargo. **S.R. Raghavan**, A. Lu

2:20 PMSE **179.** Emerging concepts in colloidal self-assembly: Rapid prototyping 3D DNA origami and self-sorting systems. **A. Walther**

2:50 Intermission.

‡ *Cooperative Cosponsorship*

3:10 PMSE **180.** Interfacial polymerization on dynamic complex colloid: Creating stabilized Janus droplets upon external perturbation. **Y. He**, S. Savagatrup, T.M. Swager

3:30 PMSE **181.** Janus polymersomes. **L. Ruiz-Perez**, C. Contini, G. Battaglia

3:50 PMSE **182.** Asymmetric polymersomes for active delivery to the brain by chemotaxis. **G. Battaglia**

Section E

Moscone Center

Esplanade Ballroom 307

Synthesis, Processing & Device Engineering of Polymeric Electronic Materials

Financially supported by Tosoh, Japan Analytical Industry (JAI) Co., Ltd

C. Di, J. Mei, *Organizers*

L. Fang, *Organizer, Presiding*

1:30 PMSE **183.** Three-dimensional, porous conjugated polymers for photocatalytic hydrogen production. **L. Yu**

2:00 PMSE **184.** Electroactive polymers for advanced energy storage devices: From synthesis to engineering. **Y. Kim**, W. Abousamra, D. Yang, O. Melton, J. Jung, S. Besic, M. Birschbach, V. Ebron, R. Mercado, P.J. Kinlen, H. Nguyen

2:20 PMSE **185.** Withdrawn.

2:35 PMSE **186.** Synthesis of long-chain acrylate copolymers for ultra-sensitive temperature sensors with wide range tunability. **F. Daigle**, K. Yang, J. Reeder, H. Handley, J. Elliott, W. Voit

2:50 PMSE **187.** Nanoconfined polymer electrolytes for rechargeable thin film lithium-ion batteries. **Z. Zhang**, J. Ding, K. Yager, B. Ocko, F. Fisher, C. Black

3:05 Intermission.

3:25 PMSE **188.** Materials for 3rd-generation solar cells based on singlet fission. **L. Campos**

3:55 PMSE **189.** Organic thin-film transistors with functionalized surface for biosensing applications. **H. Shen**, C. Di, D. Zhu

4:10 PMSE **190.** Higher hole mobility in lower-crystallinity conjugated polymers and their application to energy devices. **T. Park**

4:25 PMSE **191.** Solution-processed nanoporous organic semiconductor thin films for health and environmental monitoring. **F. Zhang**, G. Qu, E. Mohammadi, J. Mei, Y. Diao

4:40 PMSE **192.** Promising new dielectric polymers for pulsed-power high energy density capacitors using the process of rational co-design. **G.A. Sotzing**

Section F

Moscone Center

Esplanade Ballroom 308

Nanoscale Spectroscopic Characterization of Catalysts & Polymers

Infrared-Spectroscopy-Based Methods

Financially supported by Anasys Instruments, Bruker BioSpin, Bruker Nano, ExxonMobil Chemical Company, Neaspec

J. Rapp, D. Yablon, *Organizers*

P. Bao, *Presiding*

1:30 PMSE **193.** Ultra-broadband synchrotron infrared nano-spectoscopy and imaging. **H.A. Bechtel**, M.C. Martin, E. Muller, O. Khatib, M.B. Raschke

2:00 PMSE **194.** Joint nanoscale chemical-sensitive infrared imaging and mechanical property mapping of polymers at sub 20 nm spatial resolution. **X. Xu**, L. Wang, H. Wang

2:30 Intermission.

2:40 PMSE **195.** Characterization of metastable crystalline polymorphs in electrospun polymer nanofibers using AFM-IR spectroscopy and Selected Area Electron Diffraction (SAED). **J.F. Rabolt**

3:10 PMSE **196.** Developing predictive tools for onset of damage in polymer composite: Experimental insights on chemical network structure of epoxy system and its influence on mechanical performance. **D. Nepal**, J. Chalker, E. Mungall, G.S. Kedziora, A. Ecker, B. Rooths, J. Ryan, S. Barr, J. Moller, C. Kirkham, R.J. Berry, T. Breitzman

3:30 PMSE **197.** Withdrawn.

Section G

Moscone Center

Esplanade Ballroom 309

Molecular Engineering of Peptide Assembly

Drug Delivery

Financially supported by ACS Biomacromolecules

H. Cui, M. V. Tirrell, *Organizers*

A. Kros, S. L. Perry, *Organizers*, *Presiding*

1:30 PMSE **198.** Intra- and extra-cellular manipulation of cell signaling using elastin-like polypeptides. Z. Li, D. Tyrpak, M. Park, C. Lee, A. Kouhi, J. Dhandhukia, S. Hamm-Alvarez, C. Okamoto, **J.A. MacKay**

2:00 PMSE **199.** Organelle-specific subcellular delivery using mitochondria-penetrating peptides. **S.O. Kelley**

2:30 PMSE **200.** Dual-ligand peptide-functionalized liposomes targeting $\alpha_5\beta_1$ and $\alpha_6\beta_4$ integrins enhance gene delivery and selectivity to cancer cells. R.M. Levine, **E. Kokkoli**

3:00 Intermission.

3:15 PMSE **201.** Shape-changing drug carriers programmed with peptides for tissue targeting. **N.C. Gianneschi**

3:45 PMSE **202.** Enzyme-cleavable peptide amphiphiles enhance intracellular delivery. **H. Acar**, M.R. Schnorenberg, J.L. LaBelle, M.V. Tirrell

4:15 PMSE **203.** Rational design of peptide hydrogels for sustained drug delivery. **R. Hoogenboom**, A. Madder, S. Ballet

4:45 PMSE **204.** Drug-bearing supramolecular filament hydrogels. **H. Cui**

Industrial Innovations in Polymer Chemistry

Sponsored by POLY, Cosponsored by MPPG‡ and PMSE

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Industrial Chemistry: Symposium in honor of Jane Frommer

Sponsored by I&EC, Cosponsored by ANYL, BIOL, COLL, INOR, ORGN, PMSE and POLY

Advanced Materials & Technologies for Solar Energy Conversion & Storage

Sponsored by ENFL, Cosponsored by CATL, MPPG‡ and PMSE

Innovative Chemistry & Materials for Electrochemical Energy Storage

Capacitors

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

50th Anniversary Celebration of Macromolecules

Sponsored by POLY, Cosponsored by MPPG‡ and PMSE

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Supported Organometallics & Heterogeneous Catalysis

Sponsored by INOR, Cosponsored by PMSE

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

M. Grunlan, *Organizer*

8:00 - 10:00

18, 27, 29, 44, 53, 69, 78, 80, 83, 89, 94, 98, 121, 128-130, 180-181, 202. See previous listings.

206, 212, 229, 267, 270, 299, 303, 476-477, 479, 483, 488, 496, 500, 509, 511, 513, 515, 523, 532, 538, 549, 555, 557, 560, 568, 579, 584, 585, 602, 608, 611, 630-632, 635, 643, 659, 663, 688-690. See subsequent listings.

Innovating Materials for the Next Generation: Bringing Practical Applications into the Chemistry Classroom

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

TUESDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 303

Biomaterials for Immunotherapy

Z. Gu, D. J. Irvine, *Organizers*

H. Cheng, *Organizer, Presiding*

C. Jewell, Z. Liu, *Presiding*

8:30 PMSE **205.** Lymph node-targeted delivery of vaccines for cancer prophylaxis and synergistic cancer immunotherapy. **X. Chen**, G. Zhu

9:00 PMSE **206.** Engineering nanomaterial morphology to enhance immunotheranostic strategies. S. Yi, S. Allen, N. Karabin, Y. Liu, **E.A. Scott**

9:30 PMSE **207.** Ex vivo engineered immune organoids for controlled differentiation of germinal center-like B cells. **A. Singh**

10:00 Intermission.

10:15 PMSE **208.** Targeted polymeric nanoparticles: From discovery to clinical trials. **O.C. Farokhzad**

10:45 PMSE **209.** Discovery and early clinical development of Synthetic Vaccine Particles (SVP) to induce antigen-specific immune tolerance. **K. Kishimoto**

11:15 PMSE **210.** Novel polysaccharide carrier for vaccine adjuvant CpG-DNA for caner immunotherapy. **K. Sakurai**, N. Miyamoto, S. Mochizuki

11:45 PMSE **211.** Engineered polymer nanogels for lymph node restricted immune activation. **B. De Geest**

Section B

Moscone Center

Esplanade Ballroom 304

Polymers under Deformation

Structure & Morphology Changes during Deformation of Polyolefins & Polymer Composites

Cosponsored by MPPG‡ and POLY‡

Financially supported by Asylum Research, ExxonMobil Chemical Company

A. I. Norman, D. Yablon, *Organizers*

Y. Gao, *Presiding*

8:30 PMSE **212.** Deformation of amorphous, semi crystalline, and segmented polyolefin elastomers. **S. Datta**

9:00 PMSE **213.** Tensile deformation mechanism of propylene–ethylene random copolymer. J. Zhao, Y. Sun, **Y. Men**

9:30 PMSE **214.** Nanohybrid Shish-Kebab (NHSK) structure in composites of Poly(Ethylene Terephthalate) (PET) and Multiwall Carbon Nanotubes (MWCNTs). **E.L. Heeley**, D. Hughes, E. Crabb, J. Bowen, O. Bikondoa, B. Mayoral, T. McNally

10:00 Intermission .

10:10 PMSE **215.** Polymer chain stretching during uniaxial deformation: An *in-situ*, time-resolved SANS study in polymer melts. **C. Lopez-Barron**, J. Richards, Y. Zeng

10:40 PMSE **216.** Shear induced crystallization of bimodal and unimodal high density polyethylene. Y. Zhang, A.I. Norman, J. Throckmorton, A.K. Doufas, A.H. Tsou, **B.S. Hsiao**

11:10 PMSE **217.** Observations of unfolding for isotactic polypropylene under uniaxial stretching by solid-state NMR. **T. Miyoshi**

Section C

Moscone Center

Esplanade Ballroom 305

Support & Activator Effects on Metal Mediated Polymerization

Cosponsored by CATL, INOR and MPPG‡

Financially supported by ExxonMobil Chemical Company, Argonne National Laboratory

L. Luo, *Organizer*

M. Delferro, *Organizer, Presiding*

8:00 PMSE **218.** Influence of ligand structures on chromium alkene oligomerization catalysts. T. Wambach, **T.D. Tilley**

8:25 PMSE **219.** Examination of nascent polyolefin structure formed during polymerization on supported Zeigler-Natta and metallocene catalysts. **P. Brant**

8:50 PMSE **220.** Amorphous silica as a support and activator of chromium-based catalysts for olein polymerization. **S.L. Scott**, A. Fong, Y. Wang, B. Peters, A.E. Stiegman

9:15 PMSE **221.** Controlling active site formation for supported metallocene catalysts. **K.M. Clark**, A. Hock, B. Liu, W.B. Beaulieu, G.L. Glass

9:40 Intermission.

10:00 PMSE **222.** Bimetallic effects in Ni-catalyzed ethylene polymerization catalysis. **I. Tonks**, A.J. Smith, H. Chiu, R.J. Hue, E.D. Kalkman

10:25 PMSE **223.** Single-site(s) or not single-site(s): That is the question. **C. Coperet**

10:50 PMSE **224.** Alkali cations as leading actors in olefin polymerization catalysis. **L. Do**, Z. Cai, D. Xiao

11:15 PMSE **225.** Toward green olefin metathesis: Homogeneous polymer-supported ruthenium catalysts. **H. Bazzi**

Section D

Moscone Center

Esplanade Ballroom 306

Innovations in Drug Delivery Systems & Combination Products

Controlled Release

A. S. Kulshrestha, S. Sridharan, *Organizers*, *Presiding*

8:30 PMSE **226.** Withdrawn.

8:55 PMSE **227.** Small molecule responsive nanostructures for controlled drug delivery. **K. Neumann**, S. Jain, J. Geng, M. Bradley

9:20 PMSE **228.** Telodendrimers: A unique platform for engineering macromolecules based nanocarriers for tailored drug delivery. **A.K. Kakkar**

9:45 PMSE **229.** Well-defined targeted polymer-taxane prodrugs. B. De Geest, **B. Louage**

10:10 Intermission.

10:20 PMSE **230.** Sutureless wound closure with covalent controlled release for local drug delivery: Therapeutic methacrylate adhesives. Z. Wright, B. Holt, **S.A. Sydlik**

10:45 PMSE **231.** Electrically induced controlled release from biopolymer capsules. **A. Gargava**, S.R. Raghavan

Section E

Moscone Center

Esplanade Ballroom 307

Synthesis, Processing & Device Engineering of Polymeric Electronic Materials

Financially supported by Tosoh, Japan Analytical Industry (JAI) Co., Ltd

C. Di, L. Fang, J. Mei, *Organizers*

D. Lipomi, *Presiding*

8:00 PMSE **232.** High efficiency non-fullerene polymer solar cells. **S.A. Jenekhe**

8:30 PMSE **233.** Molecular engineering on conjugated side chains for high performance polymer photodetectors and solar cells. **Y. Liang**

8:50 PMSE **234.** All-polymer solar cells based on conjugated perylenediimide polymer acceptors. Y. Guo, Y. Li, H. Yan, **D. Zhao**

9:20 PMSE **235.** Highly efficient thick-film polymer solar cells. **J. Chen**

9:40 PMSE **236.** Solution-processable molecular donors & acceptors for efficient bulk-heterojunction solar cells. **P. Beaujuge**

10:00 Intermission.

10:20 PMSE **237.** Optimized alloy-parallel morphology of ternary organic solar cells. **W. Ma**

10:50 PMSE **238.** Lead perovskite formation and its application for solar cell. **Y. Guo**

11:10 PMSE **239.** Characterization of charge transport networks in non-fullerene bulk-heterojunction thin films. **M. Roders**

11:25 PMSE **240.** Multiscale simulation of solution phase behavior during organic solar cell processing. **F.L. Lee**, A.B. Farimani, K.L. Gu, H. Yan, Z. Bao, V.S. Pande

11:40 PMSE **241.** Impact of fluorination in non-fullerene acceptor organic photovoltaics. **N. Bauer**, Q. Zhang, X. Zhan, W. You

Section F

Moscone Center

Esplanade Ballroom 308

Cooperative Research Award: Symposium in honor of Paul A. Kohl & Edmund Elce

S. C. Jana, E. Reichmanis, *Organizers*, *Presiding*

8:30 PMSE **242.** Molecular engineering of anion exchange membranes for fuel cell technology application. **C. Bae**

9:00 PMSE **243.** Nanocellulose thin films and nanocellulose aerogels. A. Chang, K.L. Martin, Y. Li, **K.R. Carter**

9:30 PMSE **244.** Epoxy-based polynorbornenes for MEMS, microelectronics, and photonics. **M. Raeiszadeh**

10:00 PMSE **245.** Stable, high molecular weight polyaldehydes. **J.M. Schwartz**, O. Phillips, A. Engler, J. Lee, A. Sutlief, P. Kohl

10:30 Intermission.

10:45 PMSE **246.** Vinyl addition polymerization of norbornene monomers. Catalyst developments at Promerus LLC. **L.F. Rhodes**

11:15 PMSE **247.** Polymer dielectrics for electronic devices and packaging. **P. Kohl**, E. Elce

Section G

Moscone Center

Esplanade Ballroom 309

Molecular Engineering of Peptide Assembly

Supramolecular Assemblies

Financially supported by ACS Biomacromolecules

S. L. Perry, M. V. Tirrell, *Organizers*

H. Cui, A. Kros, *Organizers*, *Presiding*

8:15 PMSE **248.** Dipeptide-based low molecular weight gelators. E. Draper, C. Colquhoun, M. Wallace, J. Iggo, **D. Adams**

8:45 PMSE **249.** Heterotypic supramolecular assemblies of short peptidic derivatives. J. Li, **B. Xu**

9:15 PMSE **250.** Exploring the peptide sequence space for function. **R. Ulijn**

9:45 PMSE **251.** Self-assembling short peptides into complex supramolecular gels with emergent catalytic function. N. Singh, M. Araujo, **B. Escuder Gil**

10:05 Intermission.

10:20 PMSE **252.** Peptide sequence variation tunes mechanical properties and charge carrier formation within peptide-based supramolecular nanomaterials. **J.D. Tovar**

10:50 PMSE **253.** Biomolecules for non-biological things: Materials construction through peptide design and solution assembly. **D.J. Pochan**

11:20 PMSE **254.** Self-assembly of peptide amphiphiles in nonpolar solvents. **J.W. Schneider**, E. Carvalho, J. Vries, P.J. Sides, D.C. Prieve

11:50 PMSE **255.** Directing self-assembly and stability of micelles by secondary structure formation in polypeptides. **M. Barz**

Section H

Moscone Center

Esplanade Ballroom 310

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

X. Hu, F. Huang, *Presiding*

8:30 PMSE **256.** Withdrawn.

8:50 PMSE **257.** Preparation of CO_2 permeable nanomembranes from amine-containing nano-gel-particles. **Y. Hoshino**, T. Gyobu, R. Honda, K. Imamura, C. Yamashita, T. Watanabe, I. Taniguchi, Y. Miura

9:10 PMSE **258.** Programming temporal shapeshifting. **X. Hu**, J. Zhou, M. Vatankhah-Varnoosfaderani, W.F. Daniel, Q. Li, A.P. Zhushma, A. Dobrynin, S. Sheyko

9:30 PMSE **259.** Reversible photochemical control over contact electrification of polymer coatings. **X. Hu**, S.W. Thomas

9:50 PMSE **260.** Tunable non-iridescent photonic colloidsomes of bio-inspired core-shell melanin nanoparticles *via* reverse emulsion process. **Z. Hu**, M. Xiao, Z. Wang, Y. Li, M. Shawkey, A.N. Dhinojwala, N.C. Gianneschi

10:10 Intermission.

10:25 PMSE **261.** New bis-(μ-alkoxo-alkylaluminum) initiators for lactone polymerization. **C. Huang**, M. Chwatko, N.A. Lynd

10:45 PMSE **262.** Hybrid organic-inorganic multi-block 6F-DABA polyimide SiO_2-TiO_2 nanocomposites: Structure, physical properties, and gas transport. **F. Huang**, C.J. Cornelius

11:05 PMSE **263.** Fabrication of geometrically complex micro-lattices with Continuous Liquid Interface Production (CLIP) for biological applications. **R. Jansuziewicz**, C.J. Bloomquist, S.J. Mecham, J.M. Desimone

11:25 PMSE **264.** Redox exfoliation of layered transition metal dichalcogenides. **A. Jawaid**, J. Che, R.A. Vaia

11:45 PMSE **265.** Synthesis and characterization of amphiphilic brush copolymers for applications in drug delivery and as antimicrobial agents. **P. Kalelkar**, D.M. Collard

Advanced Materials & Technologies for Solar Energy Conversion & Storage

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Innovative Chemistry & Materials for Electrochemical Energy Storage

Solid-State Electrolytes & Beyond Li

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2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Conjugated Polymeric Materials

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TUESDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 303

Biomaterials for Immunotherapy

H. Cheng, *Organizer*

Z. Gu, D. J. Irvine, *Organizers*, *Presiding*

1:30 PMSE **266.** Nanoparticle mediated remodeling of the suppressive immune microenvironment in tumors. **L. Huang**

2:00 PMSE **267.** Designer vaccine nanodiscs for personalized cancer immunotherapy. **J. Moon**

2:30 PMSE **268.** Harnessing biomaterials to study and engineer lymph node function. **C. Jewell**

3:00 PMSE **269.** Engineering lymph-node targeting vaccines for type 1 diabetes. **H. Liu**

‡ *Cooperative Cosponsorship*

3:30 PMSE **270.** Macroporous scaffolds for immune cell modulation. **P. Li**, Z. Fan, H. Cheng

3:45 PMSE **271.** Manipulating immune cell responses with designer Janus interfaces. **Y. Yu**

Section B

Moscone Center

Esplanade Ballroom 304

Polymers under Deformation

Applying Advances in Characterization Methods for In-Situ Studies of Deformation

Cosponsored by MPPG‡ and POLY‡

Financially supported by Asylum Research, ExxonMobil Chemical Company

D. Yablon, *Organizer*

A. I. Norman, *Organizer, Presiding*

1:30 PMSE **272.** *In situ* TEM nanomechanical testing of polymers. **F.I. Allen**, N. Velez, M. Jones, G. Meyers, A. Minor

2:00 PMSE **273.** *In situ* morphology observations of single high-performance fibers with novel multi-axial strain approach. **K.E. Strawhecker**, M.R. Roenbeck, S. Lustig, E.J. Sandoz-Rosado

2:30 PMSE **274.** Investigating the mechanism of stress-oscillation phenomenon in a semi-crystalline biopolymer. **E.L. Heeley**, D. Hughes, E. Crabb, C. Cafolla, C. Wan

2:50 Intermission.

3:00 PMSE **275.** *In situ* Raman mapping of materials under mechanical loading: A platform for simultaneous Raman spectroscopy and nanoindentation. **C.A. Michaels**, Y. Gerbig, R.F. Cook

3:30 PMSE **276.** Development of μRheoSANS at NIST. **D. Seeman**, J. Weston, D.L. Blair, P. Salipante, S.D. Hudson, K. Weigandt

3:50 PMSE **277.** Polycaprolactone flow-induced crystallization as probed by simultaneous Raman, rheology, and optical microscopy. **A. Kotula**, K. Migler

4:10 PMSE **278.** Investigation of swelling thermodynamics of extended chain conformations within polymer thin films. **S.V. Orski**, E. Chan, K. Beers

Section C

Moscone Center

Esplanade Ballroom 305

Support & Activator Effects on Metal Mediated Polymerization

Cosponsored by CATL, INOR and MPPG‡

Financially supported by ExxonMobil Chemical Company, Argonne National Laboratory

M. Delferro, L. Luo, *Organizers*

L. Do, I. Tonks, *Presiding*

1:00 PMSE **279.** Olefin trimerization with titanium catalysts: MAO/silica-supported variants display higher productivities. **J.E. Bercaw**, D. Aluthge, A. Sattler, J.A. Labinger

1:25 PMSE **280.** Effects of activation on coordination-addition polymerization of polar vinyl monomers: From living and chemo/stereoselective to catalytic polymerization. **E.Y. Chen**

1:50 PMSE **281.** Structure-property relations of ethylene-propylene random copolymer comparison between Ziegler/Natta and self-supported single-site products. **J. Wang**, L. Boragno, L. Resconi, **M. Gahleitner**

2:15 PMSE **282.** Designing high-performance palladium and nickel catalysts for olefin polymerization and copolymerization. **C. Chen**

2:40 Intermission.

3:00 PMSE **283.** Expanding the range of polyolefin materials through Living Coordinative Chain Transfer Polymerization (LCCTP). **L.R. Sita**

3:25 PMSE **284.** Benefits from the use of cycloalkyl-bridged metallocene catalysts in ethylene polymerization. **J.M. Praetorius**, Q. Yang, C. Boxell, W.B. Beaulieu

3:50 PMSE **285.** Self-assembled multinuclear palladium catalysts for olefin polymerization. **R.F. Jordan**

4:15 PMSE **286.** Withdrawn.

Section D

Moscone Center

Esplanade Ballroom 306

Innovations in Drug Delivery Systems & Combination Products

Novel Drug Delivery

A. S. Kulshrestha, S. Sridharan, *Organizers*, *Presiding*

1:30 PMSE **287.** Efficient transdermal delivery of NSAIDS from new pressure sensitive adhesive technology (TEPI), delivery of ibuprofen, licocaine, diclofenac, etc. **D.M. Haddleton**, G. Nurumbetov, V. Nikolaou, E. Tombs

1:55 PMSE **288.** Hydrogen peroxide-activatable nanotherapeutics: Ultrasound imaging and anti-inflammatory therapy of oxidative stress-associated diseases. **D. Lee**, C. Kang, E. Jung, E. Hong, Y. Go

2:20 PMSE **289.** On the combined use of cyclodextrins and D-α-tocopheryl polyethylene glycol succinate as a drug delivery system. **G. González-Gaitano**, C. Dreiss, J. Puig

2:45 Intermission.

2:55 PMSE **290.** Enzyme-responsive nanomaterials for targeted delivery of chemo- and immunotherapeutics. **C.E. Callmann**, N.C. Gianneschi

3:20 PMSE **291.** Divided we stand: Exploiting sequogels for time-staggered delivery of dual chemotherapeutics. **P. Majumder**, U. Baxa, J. Schneider

3:45 PMSE **292.** Covalently captured dynamic self-assembled star-shaped polyglutamates as drug delivery vehicles. A. Duro-Castano, V.J. Nebot, A. Niño-Pariente, N. Feiner, J.J. Arroyo, A. Paul, A. Arminan, L. Albertazzi, **M.J. Vicent**

Section E

Moscone Center

Esplanade Ballroom 307

Synthesis, Processing & Device Engineering of Polymeric Electronic Materials

Financially supported by Tosoh, Japan Analytical Industry (JAI) Co., Ltd

C. Di, L. Fang, *Organizers*

J. Mei, *Organizer, Presiding*

1:30 PMSE **293.** Development of organic semiconducting materials for photovoltaic applications. **S.R. Marder**, J. Zhang, T. Parker, Q. Shi, S. Blakey, B. Xu, S. Agarkar, G. Pirotte, J. Reynolds, X. Zhan

2:00 PMSE **294.** Aza-Diels–Alder route to polyquinolines. **M. Umerani**, R. Kurakake, P. Patel, D.J. Dibble, R. Lopez, J.W. Ziller, A.A. Gorodetsky

2:15 PMSE **295.** Synthesis of novel quinoidal type conjugated polymers and application to organic field-effect transistors. **H. Hwang**, Y. Kim, M. Kang, K. Hwang, M. Lee, D. Kim

2:30 PMSE **296.** BDOPV-based conjugated polymers towards high performance n-type polymer field-effect transistors. **J. Pei**

3:00 PMSE **297.** Synthesis of well-defined ladder-type oligomeric *p*-phenylene derivatives via Ring-Closing olefin Metathesis (RCM). **J. Lee**, L. Fang

3:15 Intermission.

3:35 PMSE **298.** Design and synthesis of novel electron donors and acceptors for high performance organic electronic materials. **Y. Liu**, B. He, M. Kolaczkowski, L. Klivansky, T. Chen

4:05 PMSE **299.** Structure-property correlation study of quinoidal ladder oligomers and polymers. **X. Ji**, L. Fang

4:20 PMSE **300.** Generic strategy for cross-linking organic semiconducting polymer thin-films. **B. Watson**, N. Rolston, K. Bush, L. Taleghani, R. Dauskardt

4:40 PMSE **301.** New design principles for realization of high performance electrochromic materials. **G.E. Gunbas**

5:00 PMSE **302.** Innovative carboxylic acid functional propylene dioxythiophene (ProDOT-COOH) monomer for bioelectronics. **D. Mantione**, A. Sanchez-Sanchez, H. Sardon, D. Mecerreyes

Section F

Moscone Center

Esplanade Ballroom 308

Recent Advances in Multiblock Copolymers

Synthesis & Modeling

Cosponsored by POLY

Financially supported by ExxonMobil Chemical Company, The Dow Chemical Company

Z. Bai, B. K. Long, *Organizers*

J. Zhang, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 PMSE **303.** Tandem ring-opening metathesis/vinyl insertion copolymerization of ethylene with cyclic olefins: Access to functional polyolefin block-copolymers. **M. Buchmeiser**

1:35 PMSE **304.** Sequence controlled multiblock copolymers: New chemistries lead to new possibilities. **A. Anastasaki**, N. Engelis, V. Nikolaou, G. Nurumbetov, N. Truong, M. Whittaker, T. Davis, D.M. Haddleton

2:05 PMSE **305.** Synthesis of and morphological consequences of frustration in ABC and ABCA' multiblock polymers. **M.A. Hillmyer**

2:35 PMSE **306.** Fast and slow dynamical processes in simulations of block copolymer micelles. **D. Morse**, J. Mysona

3:05 Intermission.

3:25 PMSE **307.** Multiblock copolymers by ATRP. **K. Matyjaszewski**

3:55 PMSE **308.** Manipulation of effective interaction parameters from ARB and AHB type triblock copolymers. **J. Bang**, S. Woo, A. Khan, D. Ryu, S. Choi, J. Huh

4:25 PMSE **309.** Block copolymers by simultaneous copolymerisation of different monomers, unusual initiators and polymeranalogous transformations. **M. Klapper**, F. Karagoez, I. Freudensprung, K. Muellen

4:55 Concluding Remarks.

Section G

Moscone Center

Esplanade Ballroom 309

Molecular Engineering of Peptide Assembly

Helical Peptides

Financially supported by ACS Biomacromolecules

H. Cui, A. Kros, *Organizers*

S. L. Perry, M. V. Tirrell, *Organizers*, *Presiding*

1:30 PMSE **310.** Decipher 3-helix micelle as nanocarrier. **T. Xu**

2:00 PMSE **311.** Hydrophobic interactions in peptide folding, association, and assembly. **M. Shell**

2:30 PMSE **312.** Drug delivery via cell membrane fusion using lipopeptide modified liposomes. **A. Kros**

3:00 Intermission.

3:15 PMSE **313.** Collagen hybridizing peptide: Targeted binding, self-assembly, and biomedical application. **M.S. Yu**

3:45 PMSE **314.** Using molecular tuning to design functional polypeptide assemblies. **T.J. Deming**

4:15 PMSE **315.** Programmed assembly of helix bundle-forming peptide-dendron hybrids. **J.G. Rudick**

4:45 PMSE **316.** Histidine-rich amphipathic peptides exhibit a range of biological functions and self-associate into helical coiled-coil fibers and hydrogels. **B. Bechinger**, L. Vermeer, J. Wolf, A. Galy, D. Fenard

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Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

Section H

Moscone Center
Esplanade Ballroom 310

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

D. Roy, A. Shete, *Presiding*

1:30 PMSE **317.** Bactericidal and non-hemolytic macromolecules through synergistic variation in spacer arm and separate center design. **A. Punia**, K. Punia, K. Chatterjee, S. Mukherjee, J. Fata, P. Banerjee, K.S. Raja, N. Yang

1:50 PMSE **318.** Rubber toughening of photocurable resins for Continuous Liquid Interface Production (CLIP). **A.L. Quintanilla**, L. Huang, A. Nebipasagil, S.J. Mecham, J.M. Desimone

2:10 PMSE **319.** New class of organoaluminum initiators for epoxide polymerizations. **C. Rodriguez**, R.C. Ferrier, N. Lynd

2:30 PMSE **320.** Effect of CNCs on crystallization kinetics of polycaprolactone as probed by Rheo-Raman microscopy. **D. Roy**, A. Kotula, D. Fox, K. Migler, J. Gilman, B. Natarajan

2:50 PMSE **321.** Vat photopolymerization additive manufacturing for the construction of graded and multi-material objects. **J. Schwartz**, C. Thrasher, A.J. Boydston

3:10 Intermission.

3:25 PMSE **322.** Weld formation in polymer extrusion additive manufactuing processes. **J. Seppala**, S. Hoon Han, K.E. Hillgartner, C.S. Davis, K. Migler

3:45 PMSE **323.** Understanding moisture outgassing kinetics of a silica reinforced polydimethylsiloxane using experimental and first-principles modeling. **H. Sharma**, W. McLean II, R.S. Maxwell, L. Dinh

4:05 PMSE **324.** Polymer gel electrolytes with jeffamine-amine coupled polyureas structure for enhancing efficiency of dye-sensitized solar cells. **S. Shen**, P. Shih, K. Ho, J. Lin

4:25 PMSE **325.** One-pot blue-light triggered Interpenetrating Polymeric Network (IPN) from rapid CuAAC and methacrylate reactions with superior mechanical properties. **A. Shete**, C.J. Kloxin

4:45 PMSE **326.** Preventing blood loss with self-sealing hemostatic needles. **M. Shin**, H. Lee

Advances in Polysaccharides: Practice & Applications

New Developments in the Industrial Sector

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Advanced Materials & Technologies for Solar Energy Conversion & Storage

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Innovative Chemistry & Materials for Electrochemical Energy Storage

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Materials for Energy Conversion

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TUESDAY EVENING

Section A

Moscone Center
Hall A

Joint PMSE/POLY Poster Session

M. Grunlan, *Organizer*

6:00 - 8:00

General Posters/New Concepts in Polymeric Materials.

PMSE **327.** Photo-controlled proton transfer in polymer films using metastable-state photoacids. **N. Abeyrathna**, C. Yang, T. Khalil, Y. Liao

PMSE **328.** Tuning interfacial energy of nanodiamond fillers for property reinforcement in polymer nanofiber composites. **P. Adhikari**, S.A. Khan, O.J. Rojas

PMSE **329.** Synthesis of fluorescent phenyleneethynylene trimer-containing polymer. **M. Ahmed**, J. Moon

PMSE **330.** Heteroarm core cross-linked star polymers via RAFT alternating copolymerization. **N. Ahn**, M. Seo

PMSE **331.** Preparation and structural studies of electrospun polyvinyl alcohol/Ru_2S_3 and hydroxylethyl/Ru_2S_3 nanofibers. **P.A. Ajibade**

PMSE **332.** High loaded sulfur – polymer/graphene cathode material for Li-S batteries. A. Abraham, V. Pillai, S. Lonkar, **S. Al Hassan**

PMSE **333.** Tunable hygromorphism: Structural implications of low molecular weight gels and electrospun nanofibers in bilayer composites. **S. Alexander**, L.T. Korley

PMSE **334.** Synthesis and developing properties of functional phenolic polymers for eco-friendly thermal printing papers. **B. An**, K. Choi, H. Kwon, Y. Ryu

PMSE **335.** High performance electrochromic material shows voltage-dependent fluorescence change. **G. Atakan**, Y. Arslan Udum, G.E. Gunbas

PMSE **336.** Device physics of the organic alloying effect in high-efficiency ternary blend polymer/fullerene bulk-heterojunction solar cells. **T. Aubry**, B.J. Schwartz

PMSE **337.** Performance of liquid benzoxazine-PEG blend resin systems for potential industrial composites processing. **E. Brown**, D.A. Rider

PMSE **338.** Novel comonomers for highly branched LDPE. **H.A. Brown**, M. Demirors, C. Eddy, S. Ewart, J. Osby

PMSE **339.** Dimeric drug polymeric nanoparticles with exceptionally high drug loading and quantitative loading efficiency. **K. Cai**, J. Cheng

PMSE **340.** Production and characterization of microbial polyhydroxyalkanoates. **A. Cal**, D. Sikkema, M. Ponce, W.J. Orts, C. Lee

PMSE **341.** Architectural influence on the assembly of biosynthetic polymer analogues to a peptide hydrogel. **A.S. Carlini**, D.T. Crystal, S. Sahu, F.J. Hidalgo, A.P. Blum, N.C. Gianneschi

PMSE **342.** Metal-containing polyesters from 3,5-pyridinedicarboxylic acid, 2-ketroglutaric acid, dipicolinic acid, and camphoric acid. **C.E. Carraher**, M. Roner, P. Slawek, F. Mosca, D. Patel, K. Black, J. Einkauf, F. Russell, J. Frank, A. Moric-Johnson, L. Miller, L. Chen

PMSE **343.** Synthesis of metallocene-containing polyethers. **C.E. Carraher**, M. Roner, K. Black, J. Frank

PMSE **344.** Development of *Aloe vera*/violet silver nanoparticles/bacterial cellulose film for using as burn wound dressings. **L. Chatchawanwirote**

PMSE **345.** Fully physically-linked hydrogels with superior mechanical, self-healing, and antifouling properties. **H. Chen**, Q. Chen, F. Yang, K. Chu, R. Hu, M. Zhang, B. Ren, J. Zheng

PMSE **346.** Reduced confinement and its effect on stability in strong polyelectrolyte brushes. **W. Chen**, M. Menzel, T. Watanabe, O. Prucker, J. Ruehe, C.K. Ober

PMSE **347.** Effect of oligomeric resin on silica-filled rubber compound. **Y. Chen**, Y. Liu, F. Lo, Z. Zheng, C. Hsieh, C. Dai

PMSE **348.** Withdrawn.

PMSE **349.** Modified Stöber method for the synthesis of dextran-SiO_2 glyconanoparticles for siRNA delivery. **O.M. Chesniak**, D. Vocelle, C. Chan, S. Walton, M.R. Smith

PMSE **350.** Synthesis and characterization of indolocarbazole pyrroledione-based organic semiconductors. **K. Choi**, J. Park, J. Kwon, Y. Ryu, B. An, S.Y. Park

PMSE **351.** Fabrication of Pickering emulsion stabilized by associative magnetic nanoparticles for recoverable emulsion flooding. **S. Choi**, J. Kim

PMSE **352.** Biodegradable hairy nanoparticles for biomedical applications. **S. Christau**, J. Lahann

PMSE **353.** Preparation and characterization of hydrogel wound dressing loaded PLGA/white thyme oil PLGA nanospheres for used as pressure ulcer treatment. **C. Choipang**, O. Suwantong, P. Chuysinuan, P. Ekabutr, P. Supapol

PMSE **354.** Design of electronically-active polyionenes at organic/inorganic interfaces. **M.D. Cole**, M. Sheri, C. Bielicki, T. Emrick

PMSE **355.** Development of double layer-wound dressing of biopolymer containing rice extract and essential oil for biomedical applications. **P. Chuysinuan**, N. Chimnoi, A. Makarasen, N. Reuk-ngam, L. Pattani, P. Khlaychan, S. Techasakul

PMSE **356.** Monomer encapsulated ARGET ATRP emulsion polymerization for synthesis of Polymer-Grafted Nanoparticles (PGNs). **R. Cordero**, C.K. Ober, R.A. Vaia

PMSE **357.** Morphology and responsive properties of mosaic polymer brushes. **O. Davydovich**, E. Chu, P.B. Moore, A. Sidorenko

PMSE **358.** Synthesis of latexes from plant oil-based acrylic monomers. **Z. Demchuk**, I. Tarnavchyk, V. Kirianchuk, A.S. Voronov

PMSE **359.** Induction of adipose-derived stem cells on nanofibrous, porous microspheres for vascularized adipose tissue regeneration *in vivo*. **Y.R. Doleyres**, J. Wang, X. Jin, P.X. Ma

PMSE **360.** Preparation and characterization of a nano-composite constrained high temperature drilling fluid with water soluble AM-SAS-SSS copolymers by inverse microemulsion polymerization. **Q. Deng**, **Y. Ke**

PMSE **361.** Self-healing poly(hydroxyalkanoates) formed from metal-ligand complexation. **T. Ebrahimi**, S. Hatzikiriakos, P. Mehrkhodavandi

PMSE **362.** Synthesis and characterization of Polycaprolactone (PCL) membranes as scaffolds for bone tissue engineering. **E.A. Dwomoh**, J. Santillan, E.O. Ortiz-Quiles, E. Nicolau

PMSE **363.** Biologically relevant polymeric materials based on the azobenzene motif. **T. Eom**, Y. Lee, S. Kim, J. Bang, A. Khan

PMSE **364.** Laminar flow-based fabrication of thin film battery separators from aramid nanofibers. **A.E. Emre**, P. Weerappuli, S. Takayama, N. Kotov

PMSE **365.** Understanding ordering of block-copolymer-based supramolecules on lithographically patterned surfaces. **K. Evans**, T. Xu

PMSE **366.** Advanced polymer nanocomposites for 3D printing in space. **C. Fincher**, Y. Mizuno, G. Garner, T. Ozkan, J. Meyer

PMSE **367.** Synthesis, characterization and gas transport properties of Tröger's Base-Based Polyimides of Intrinsic Microporosity (TB-PIM-PIs). **B. Ghanem**, N. Alaslai, I. Pinnau

PMSE **368.** Selective a-olefin oligomerization using group IV amine bis(phenolate) catalysts. **T.N. Gunasekara**, M.M. Abu-Omar

PMSE **369.** Near infrared responsive hydrogels with fast and spatially controlled responses. **I.M. Hill**

PMSE **370.** Tailoring multi-site catalysts and in-situ formation of self-reinforcing all-polyolefin composites for sustainable light-weight construction. **T. Hees**, M. Stürzel, R. Mülhaupt

PMSE **371.** Material design for perovskite solar cell. **C. Holmes**, O. Allam, Z. Greenberg, S. Jang, K. Kim

PMSE **372.** Enhancement of elasticity in alginate-clay nanocomposite hydrogels with PEO-PPO-PEO copolymers. **W. Hom**, S.R. Bhatia

PMSE **373.** Stimuli-sensitive lipid coated nanogels (lipogels) for hydrophilic and hydrophobic guest delivery. **C. Homyak**, S. Thayumanavan

PMSE **374.** Single component hydrogel simultaneously exhibiting stretchable, self-healing, stimuli-responsible, and adhesive properties. **S. Hong**, H. Lee

PMSE **375.** Withdrawn.

PMSE **376.** Morphology and adsorption kinetics of 0D, 1D, and 2D carbonaceous nanomaterial networks in polymeric electrospun fibers. **N. Hoogesteijn von Reitzenstein**, O. Apul, E.L. Pruitt, K. Hristovski, P.K. Westerhoff

PMSE **377.** Incorporation of nile red in hyperbranched poly n-isopropylacrylamide and its response to environmental change. **R. Hoskins**, S. Rimmer

PMSE **378.** Hybrid organic-inorganic polyimide SiO_2-TiO_2 nanocomposites: Structure, physical properties, and gas seperation. **F. Huang**, C.J. Cornelius

‡ *Cooperative Cosponsorship*

PMSE **379.** Synthesis of a dendritic scaffold that will be used for antioxidant dendrimer synthesis. **U.G. Huynh**, C.Y. Lee

PMSE **380.** Chemosensor of Nile Red deposition in poly(styrene-co-maleic anyhydride) core-shell for copper cation in water. **K. Hwang**, J. Park, J. Lee

PMSE **381.** Carbon dioxide gas indicating film using the hydrophobic ion pair dye doped on polyethyleneimine/poly(styrene-co-maleic anhydride). **K. Hwang**, W. Choi, J. Lee

PMSE **382.** Synthesis of various cycloaliphatic polyester copolymers based on Poly(1,4-cyclohexylidenecyclohexane-1,4-dicarboxylate) (PCCD) with tunable glass transition temperature and viscosity using melt polymerization technique. **S. Ikikardesler**, **R. Piyade**, A.E. Acar

PMSE **383.** One-step fabrication of multi-scale diffractive gratings by directional photofluidized surface relief of azo polymers. **Y. Jeong**

PMSE **384.** Preferential ordering of poly(3-hexylthiophene) on two type graphene substrates. **K. Jo**, S. Chae, J. Choi, S. Won, J. Kim, H. Kim

PMSE **385.** Structural characterization of three-helix micelle delivery platform for neurological disease treatment. **B. Jung**, J. Ang, T. Xu

PMSE **386.** Development of chitosan derivatives/starch foam for use as oral surgical wound dressing. **N. Jungprasertchai**

PMSE **387.** Synthesis of cycloaliphatic polyesters, poly(1,4-cyclohexylidenecyclohexane- 1,4-dicarboxylate) (PCCD), for low temperature curing powder coatings. **K. Kalayci**, **R. Piyade**, **B. Salman**, A.E. Acar

PMSE **388.** Adhesion control of polymeric dry adhesives using partial wrinkle generation method. **S. Kang**

PMSE **389.** Withdrawn.

PMSE **390.** Microfluidic synthesis of uniform gelatin microparticles for temporary embolization. **B. Kim**, S. Choi, S. Han, J. Kim

PMSE **391.** Stimuli-responsive release of guests from mesoporous nanocontainer induced by conformational conversion of peptide gatekeepers. J. Lee, **C. Kim**

PMSE **392.** Surface modification of microcrystalline cellulose to capture CO2 as fillers in LDPE composite. K. Ha, **H. Kim**, S. Park, Y. Yang

PMSE **393.** Thermal stability and physical properties of basalt fiber reinforced epoxy composite modified by silane coupling agents. **H. Kim**, J. Lee, I. Nam

PMSE **394.** Fluorescent supracolloidal chains of diblock copolymer micelles with color tunability. **K. Kim**, S. Jang, B. Sohn

PMSE **395.** Fabrication of methacrylated silk fibroin hydrogel by photo-cross-linking. **M. Kim**, H. Kim, Y. Park, C. Ki

PMSE **396.** Effect of plant oil unsaturation on emulsion copolymerization with vinyl monomers. **K. Kingsley**, O. Shevchuk, I. Tarnavchyk, A. Voronov

PMSE **397.** Chemical warfare agent simulant sensing via natural polymeric photonic crystals. **J. Kittle**

PMSE **398.** Synthesis of amphiphilic PEO-b-PCL-b-PEO triblock copolymers as novel polymeric surfactants. **J. Lee**, H. Seo, J. Kim

PMSE **399.** Withdrawn.

PMSE **400.** Optimization of electrochromics on polycarbonate substrates: Use of thermal and long wavelength photo-initiators. **M. Li**, x. zhang, G.A. Sotzing

PMSE **401.** Preparation and characterization of a novel halogen-free flame retarded polyamide 6. **K. Liu**, Y. Li, R. Xiao

PMSE **402.** MOF-random copolymer nanocomposite. **S. Liu**, T. Xu

PMSE **403.** Dynamic mechanical behavior of thermoset rubber blends. **Y. Liu**, Y. Chen, J. Wang, H. Lin, C. Dai, C. Hsieh

PMSE **404.** Graphene/polyanilne blended fiber for conducting and flexible energy storage devices. Y. Feng, J. Shen, C. Ma, D. Zhang, Z. Xiao, **Y. Liu**, **Y. Min**

PMSE **405.** Synthesis of graft copolymers with N-vinylimidazole onto pristine and modified polypropylene monofilaments: PP-g-PNVIm, (PP-g-PHEMA)-g-PNVIm, and (PP-g-PNIPAAm)-g-PNVIm. **F. Lopez Saucedo**, **E. Bucio**

PMSE **406.** Enzyme induced mineralization of hydrogels. **M. Meuris**, N. Rauner, J.C. Tiller

PMSE **407.** Polymer thin film surfaces for molecular transport and concentration. **K.A. Miller**, L. Kisley, P.V. Braun

PMSE **408.** Relationship between cure temperature and the mechanical, physical, and dielectric performance of a polydimethylsiloxane/glass composite for electric motor insulation. **S. Miller**, K. Becker, T. Williams, D. Scheiman, P. Heimann, A. Ring

PMSE **409.** Physical, thermal, electrochemical and fuel cell performance study of sulfonated poly(phenelyne)s/novel branched polysulfone-based polymer blend. **B. Motealleh**, T.D. Largier, F. Huang, C.J. Cornelius

PMSE **410.** Imprinted polymeric materials for selective recognition of anti-diabetic drugs in complex mixtures. **A. Mujahid**, I. Haq, T. Hussain, S. Bajwa

PMSE **411.** Zinc and cadmium coordination polymers of aliphatic systems as dielectric materials. **S. Nasreen**, M.L. Baczkowski, G.M. Treich, A. Mannodi-Kanakkithodi, S.K. Scheirey, R. Ramprasad, G.A. Sotzing

PMSE **412.** Agarose coating to combat peritoneal dialysis catheter-associated complications. **K. Neoh**, M. Li, J. Rahmat, K. Mandakhalikar, E. Kang, E. Chiong

PMSE **413.** Synthesis and characterization of copolymers of β,β′- branched alkyl fused thiophenes with branched alkyl diketopyrrolopyrrole. **W. Niu**, A. Wallace, J.R. Matthews, M. He

PMSE **414.** UV-curable flame retardant coatings for cotton fabrics. Z. Yildiz, **H. Onen**, A. Gungor, Y. Wang, K. Jacob

PMSE **415.** Effect of catalyst concentration on acid-epoxy reactions: A powder coating study. **A. Ozdemir**, A. Ozcan, B. Salman, A.E. Acar

PMSE **416.** Catalyst screening for powder coating by differential scanning calorimetry. **A. Ozdemir**, **A. Ozcan**, A.E. Acar

PMSE **417.** Withdrawn.

PMSE **418.** Optimizing parameters for electrospinning alginate- and chitosan-based nanofibers. **K. Penton**, W. Weeks, T. Brown, S.K. Hamilton

PMSE **419.** Physical and chemical analysis of photodegraded high-density polyethylene by natural and accelerated ultraviolet light exposure. **L.N. Perry**, D. Stanley, H. Hsueh, J. Kim, D.L. Hunston, C.C. White, L. Sung

PMSE **420.** Janus dendrimer from poly(aryl ether) linked PAMAM for supergelation and guest release. **P. Prabakaran**

PMSE **421.** Curcumin-glucose macromolecular conjugates via click-chemistry for selective chelation of toxic metals. **K. Punia**, A. Averick, A. Punia, S. Dolai, S.R. Guariglia, W. L'Amoreaux, K.S. Raja

PMSE **422.** Increase in compatibilization of engineered resins with modified polyolefins. **R. Putans**, Q. Wan, B. Walther, E. Keene, Y. Li, M. Williams

PMSE **423.** Enhancement of binding affinity of catechol and catecholic polymer to 4-fluorophenylboronic acid through nitration of aromatic ring. **S. Qiu**, S. Jin, N. Yang

PMSE **424.** Protein surface PEGylation for the emulsion-based formation of stable nanoparticles. **L. Radi**, M. Fach, E. Steiert, P. Wich

PMSE **425.** Novel properties of polymers upon critical cross-linking right at the borderline between thermoplastic and elastomer. **T. Raidt**, F. Katzenberg, J.C. Tiller

PMSE **426.** Light-activated non-equilibrium processes at the interface of a nanoassembly. **P. Rangadurai**, S. Thayumanavan, M. Molla, J.J. De Pablo

PMSE **427.** Graphene oxide armored polythioether particles. **B. Rodier**, E. Mosher, S. Burton, R. Matthews, E. Pentzer

PMSE **428.** In situ synthesis of conductive polymers within covalent organic frameworks. **N. Sahiner**, S. Demirci

PMSE **429.** Photomediated approach for patterned bottlebrush networks. **C. Sample**, E. Discekici, N. Dolinski, D. Lunn, A. Anastasaki, C.J. Hawker

PMSE **430.** Charge transfer modulated self-assembly in poly (aryl) ether dendron derivatives with improved stability and transport characteristics. **S. Satapathy**

PMSE **431.** Polymer antibiotic conjugates based on poly(2-oxazoline)s. **M. Schmidt**, C. Krumm, J.C. Tiller

PMSE **432.** Understanding the relationship between semiconducting polymer crystallinity and the electrical properties of sequentially-processed F4TCNQ-doped P3HT films. **D.T. Scholes**, P. Yee, S.A. Hawks, J. Lindemuth, S.H. Tolbert, B.J. Schwartz

PMSE **433.** New approach to fabricate thermally responsive nanoscale emulsion films by layer-by-layer deposition. **H. Seo**, J. Lee, J. Kim

PMSE **434.** CO_2-sensitive poly(*N*-isopropylacryl amide-co-acrylic acid) copolymers with high glass transition temperatures. **Y. Shieh**, P. Lin

PMSE **435.** Fabrication of superhydrophobic coatings on AA 6061. **N.A. Siddiqui**, A. Zeeshan, H. Haseeb, M. Shaharyar

PMSE **436.** Functionalized nanofiber scaffolds for neural differentiation of mouse ESCs. **E. Silantyeva**, J. Carpenter, W. Nasir, R. Willits, M. Becker

PMSE **437.** Continuous Electrocardiogram (ECG) measurement via optimization of electrochemical state of a conductive polymer on fabric. **S.K. Sinha**, Y. Noh, G.M. Treich, S.H. Alipour, K.H. Chon, G.A. Sotzing

PMSE **438.** Super oxygen and improved water vapor barrier of polypropylene film with polyelectrolyte multilayer nanocoatings. **Y. Song**, P. Tzeng, J.C. Grunlan

PMSE **439.** Preparation of surfactant-resistant polymersomes with ultra-thick membranes through RAFT dispersion polymerization. **Z. Song**, Y. Huang, V. Prasad, R. Baumgartner, S. Zhang, K. Harris, J.S. Katz, J. Cheng

PMSE **440.** Glycocalyx-inspired nitric oxide-releasing polysaccharide coating on TiO_2 nanotube surfaces reduce platelet adhesion and activation. **J. Staver**, R. Simon-Walker, R. Romero, Y. Zang, M.M. Reynolds, K. Popat, M. Kipper

PMSE **441.** Facile approach to large-scale and three-dimentional pore-forming on polymeric objects. J. Huang, **W. Sun**

PMSE **442.** Withdrawn.

PMSE **443.** Snatching bacteria out of biofilms using the power of polymer desolvation. **T. Swift**, R. Plenderleith, S. Rimmer

PMSE **444.** Fabrication and characterization of thiol-norbornene schizophyllan hydrogels. **H. Tae**, S. Lee, M. Kim, C. Ki

PMSE **445.** Preparation and characterization of full biobased polyamide 109 based on the renewable monomer: Application in engineering thermoplastics. **L. Tao**, R. Xiao

PMSE **446.** Effect of multi-branched PDLA additives on the mechanical and thermomechanical properties of blends with PLLA. **L.F. Torres**, C. Mcmahan, W.J. Orts

PMSE **447.** Control of graphene at the interface of the polyethylene/polypropylene blends: Fabricated conductive composites with ultralow percolation thresholds. **C. Tu**, K. Nagata, M. Higuchi

PMSE **448.** Aramid nanofiber films for ionizing radiation detection via semiconducting nanoparticles. **D. Vecchio**, B. Davis, M. Hammig, N. Kotov

PMSE **449.** Photophysics of polarons and bipolarons in F4TCNQ-doped semiconducting polymers. **M.G. Voss**, D.T. Scholes, J. Challa, J. Lindemuth, B.J. Schwartz

PMSE **450.** Convenient one-step preparation of isoporous nanostructures by melt-shear organization. **S. Vowinkel**, M. Gallei

PMSE **451.** Modifying PDMS surface using infiltration interfacial polymerization. **M. Wang**, J.M. Gorham, J. Killgore, F. DelRio, Z. Zhang, Y. Ding

PMSE **452.** New polyolefins via ring-opening metathesis polymerization for biomedical applications. **Y. Wang**, M.A. Hillmyer

PMSE **453.** Homoporous structures derived from amphiphilic block copolymers. **Y. Wang**

PMSE **454.** PEG-polypeptide dual brush block copolymers. **Z. Wang**, J. Cheng

PMSE **455.** Responsive nanoporous membranes by selective swelling of triblock terpolymers. **Y. Wang**, **Z. Wang**

PMSE **456.** Towards fibers that will possess hydrophobic/oleophpbic properties for an extended period of time. **L. Wei**, T. Demir, P. Brown, I.A. Luzinov

PMSE **457.** Modified biopolymers as dynamic materials for nanoparticulate drug delivery. D. Bamberger, M. Fach, L. Radi, **P.R. Wich**

PMSE **458.** Iron(II) crosslinked bipyridine-terminated poly(dimethylsiloxane) as an elastomer. **Z. Williams**, E. Burwell, A. Chiomento, J. Pawlik, A.D. Schwab, M.S. Hambourger

PMSE **459.** Withdrawn.

PMSE **460.** Super-wettability based fabrication of one-dimensional materials. **Y. Wu**, L. Jiang

PMSE **461.** Zwitterionic polymer brushes for salt-responsive polymer structure-surface activity relationship. **S. Xiao**, H. Chen, R. Hu, M. Zhang, B. Ren, F. Yang, K. Chu, J. Yang, J. Zheng

PMSE **462.** Large nanoparticle assembly in block copolymer-based supramolecule. **Y. Xiao**, T. Xu

PMSE **463.** Effect of weight ratios of PHBV/PLA polymer blends on nitrate removal efficiency and microbial community during solid-phase denitrification. **Z. Xu**

PMSE **464.** Synthesis and characterization of ultralow fouling poly(N-acryloylglycinamide) brushes. **F. Yang**, H. Chen, Q. Chen, K. Chu, R. Hu, M. Zhang, B. Ren, J. Zheng

PMSE **465.** Effects of silane surface treatment of microcrystalline cellulose on mechanical properties of polyurethane composites. K. Ha, **Y. Yang**, H. Kim, S. Park, K. Lim

PMSE **466.** Study on the functional effect of nano composites lubricant and lubricating drilling fluid. **C. Yu**, **Y. Ke**

PMSE **467.** Cationic conjugated polymers for discrimination of microbial pathogens. **H. Yuan**

PMSE **468.** Uniaxial stretching induced packing and folding structure change in isotactic polypropylene. **S. Yuan**, T. Miyoshi

PMSE **469.** Next generation semiconducting carbonaceous material, graphyne: Its synthesis, properties and electrical applications. **E. Yun**, S. Cho, D. Ryu, H. Lee

PMSE **470.** Effect of temperature and concentration on self-assembly and mechanical properties of triblock copolymer gels. **M. Zabet**, S. Mishra, S. Kundu

PMSE **471.** Membrane gas separation accelerated by hollow nanospheres. **J. Zhang**, S.M. Mahurin, S. Dai

PMSE **472.** Neutral color tuning of flexible conjugated polymer electrochromic devices achieved by multi-component systems. **X. Zhang**, M. Li, G.A. Sotzing

PMSE **473.** Polymer-aided rituximab-epirubicin conjugate for treatment of B-cell malignancies. **L. Zhang**, **Y. Fang**, J. Kopecek, J. Yang

PMSE **474.** Mixed micellar assembles as polymer adjuvants for peptide administration. **O. Zholobko**, A. Kohut, S. Stafslien, L. Vanderwal, A.S. Voronov

PMSE **475.** Multi-stimuli-responsive amphiphilic assemblies through simple postpolymerization modifications. **J. Ziwen**, X. Liu, S. Thayumanavan

Molecular Engineering of Peptide Assembly.

PMSE **476.** Controlled synthesis of high molecular weight polypeptides. **R. Baumgartner**, H. Fu, Z. Song, Y. Lin, J. Cheng

PMSE **477.** Injectable cyclic peptide pro-gelators as enzyme-responsive hydrogels for post-myocardial infarction tissue engineering. **A.S. Carlini**, N.C. Gianneschi

PMSE **478.** Water-soluble Au(I)-phosphane complexes: From post-modification of biomolecules to peptidic self-assembly into fluorescent micelles. **B. Kemper**, P. Besenius

PMSE **479.** Controlling size, shape and function of core cross-linked nanostructures: Exploiting secondary structure in reactive polypept(o)ides to direct self-assembly. **K. Klinker**, O. Schäfer, D. Huesmann, L. Braun, L. Capelôa, M. Barz

PMSE **480.** Amino acid-encoded transient helicity by biocatalytic self-assembly. **M. Kumar**, R. Ulijn

PMSE **481.** Biomimetic approach to engineering high affinity protein-binding supramolecular nanofibers. **Y. Li**, L. Lock, Y. Wang, X. Xu, Z. Li, H. Cui

PMSE **482.** Peptide-Oligonucleotide Chimeras (POCs): Programmable building blocks for the construction of soft nanoscale matter. **A. Merg**, R. Thaner, S. Mokashi Punekar, S.T. Nguyen, N.L. Rosi

PMSE **483.** Biologically active peptide quaternary structures with topological diversity using orthogonal, abiotic dynamic covalent reactions. **J.F. Reuther**, I. Kolesnichenko, E.T. Hernandez, D.V. Ukraintsev, E.V. Anslyn

PMSE **484.** Withdrawn.

Recent Advances in Multiblock Copolymers.

PMSE **485.** Withdrawn.

PMSE **486.** Graded, hierarchically porous carbon materials from block copolymer and organic additive co-assembly. **S.A. Hesse**, J. Werner, P. Beaucage, K. Barteau, U.B. Wiesner

PMSE **487.** Janus container. **F. Liang**

PMSE **488.** Elaboration of photoreversible poly(ε-caprolactone)-based networks with two-way shape-memory effect. **F. Pilate**, R. Mincheva, L. Wu, J. Raquez, P. Dubois

PMSE **489.** Video-rate AFM imaging of block copolymer evolution. **J.G. Raybin**, J. Ren, P.F. Nealey, S.J. Sibener

PMSE **490.** Polymersome membrane-confined self-assembly. **L. Ruiz-Perez**, L. Messager, J. Gaitzsch, A.S. Joseph, L. Sutto, F. Gervasio, G. Battaglia

PMSE **491.** Development of engineered bionanomaterial based on dispersed nanodiamonds into self-assembled polystyrene-block-poly(ethylene oxide) copolymer. **J. Santillan**, Y. Rodríguez, S.A. Bello, E. Nicolau

PMSE **492.** Transient network formed by supramolecular assembly of oligocarbonate-fluorene end-functionalized poly(ethylene glycol). **G. Wei**, S. Ali, V.M. Prabhu, S. Venkataraman, Y. Yang, J. Hedrick

PMSE **493.** Microscopic structures in ion exchange fuel cell membranes. **J. Lu**, A. Spakowitz, C. Frank, M. Toney

Synthesis, Processing & Device Engineering of Polymeric Electronic Materials.

PMSE **494.** Effects of network termination on elastic and thermal expansion asymmetries in hybrid molecular materials. **J. Burg**, R. Dauskardt

PMSE **495.** Correlating radiative dynamics with structural heterogeneity in conjugated polymers. **W.R. Hollingsworth**, J. Lee, L. Fang, A. Ayzner

1D Nanomaterials: Synthesis, Assembly, Properties & Applications.

PMSE **496.** Dual modal nanosensors for the early detection of *Escherichia coli* O157:H7. **T. Banerjee**, S. Sulthana, T. Shelby, J.G. McAfee, S. Santra

PMSE **497.** Gradient structure nanofibrous assemblies for broadband acoustic absorption. **L. Cao**, J. Yu, B. Ding

PMSE **498.** Versatile stimuli-responsive ROMP-based polymeric system for modulating orientation of liquid crystal microdroplets. **Y. Huang**, Y. Kim, N.C. Gianneschi, N.L. Abbott

PMSE **499.** Aligned silver nanowire transparent electrodes for flexible electronic devices. **S. Kang**, S. Cho, H. Ko

PMSE **500.** Role of phenolic compounds in the formation of fluorescent carbon nanoparticles from natural polysaccharides. **K. Lee**, E. Park, C. Jeong, S. Park, H. Lee

PMSE **501.** Electret polyvinylidene fluoride nanofibers hybridized by polytetrafluoroethylene nanoparticles for high-efficiency air filtration. **L. Yuyao**, X. Zhao, J. Yu, B. Ding

PMSE **502.** Layer-by-layer assembly and spectroelectrochemical study of alizarin red S-based thin films. **W. Ma**, J. Lutkenhaus

PMSE **503.** Polymerization of 3,4-ethylenedioxythiophene in CD-MOF. **W. Michida**, A. Nagai, M. Sakuragi, K. Kusakabe

PMSE **504.** Nanoribbons and nanofractals self-assembled from graphene quantum dots. **Z. Qu**, W. Feng, N. Kotov

PMSE **505.** Development of designer nanomedicines and nanosensors: Important roles in human health. **S. Santra**, T. Banerjee, T. Shelby, S. Sulthana, J.G. McAfee, I.S. Zegar

PMSE **506.** Hierarchically structured superhydrophobic and superoleophilic nanofibrous membranes for effective oil-water separation. **F. Wang**, L. Huang, B. Ding

PMSE **507.** Hydrophobic polyvinylidene fluoride fibrous membranes with simultaneously water/windproof and breathable performance. **X. Yu**, Y. Li, X. Wang, B. Ding

PMSE **508.** Polyurethane/fluorinated polyurethane membranes with waterproof and breathable performance improved by lithium chloride. **J. Zhao**, Y. Li, L. Liu, B. Ding

Innovations in Drug Delivery Systems & Combination Products.

PMSE **509.** Polypept(o)ides: From polymers based on endogenous amino acids to therapeutics and imaging agents. **M. Barz**

PMSE **510.** Controllable multi-compartmental capsules with distinct cores and shells for synergistic release. **F. He**, **W. Wang**, **X. He**, **X. Yang**, **M. Li**, **R. Xie**, **X. Ju**, **Z. Liu**, **L. Chu**

PMSE **511.** PEG architecture effect on the hybridization thermodynamics and protein accessibility of PEGylated oligonucleotides. **F. Jia**, X. Lu, X. Tan, K. Zhang

PMSE **512.** Transiently responsive block copolymer micelles based on (meth)acrylamides engineered with hydrolyzable carbonate side chains. B. De Geest, **S. Kasmi**

PMSE **513.** Protein-induced supramolecular disassembly of amphiphilic polypeptide nanoassemblies. M. Molla, **P. Prasad**, S. Thayumanavan

PMSE **514.** Tuning cell behaviour by nanoparticles shape. **L. Rizzello**, A.S. Joseph, C. De Pace, G. Battaglia

PMSE **515.** Micellar thrombin-binding aptamers as reversible nanoscale anticoagulants. **A. Roloff**, A.S. Carlini, N.C. Gianneschi

PMSE **516.** Light activation and triggered drug release of multi-agent loaded nanoconstructs for simultaneous suppression of multiple treatment escape pathways in the pancreatic cancer. **B.B. Sears**, B.Q. Spring, L. Zheng, T. Hasan

PMSE **517.** Dendrimer-modified MoS_2 nanoflowers for combinational gene silencing and photothermal therapy of tumors. **X. Shi**, L. Kong, L. Xing, C. Alves, L. Du

PMSE **518.** Drug-eluting magneto-fluorescent nanoparticles for combined imaging and therapy. **A. Simchi**, **Y. Wang**

PMSE **519.** Engineering the local lymph node microenvironment to promote immunological tolerance. **L.H. Tostanoski**, T. Simon, J. Bromberg, C. Jewell

PMSE **520.** Self-assembled transferrin-polymer conjugate nanocarriers for the delivery of therapeutics. **A. Wong**, A.P. Johnston, G.K. Such

PMSE **521.** Helical antimicrobial polypeptides with radial amphiphilicity. **M. Xiong**, J. Cheng

PMSE **522.** Enteric elastomer enables safe gastric retention and extended oral drug delivery for improved medication adherence. **S. Zhang**, R.S. Langer

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Sponsored by POLY, Cosponsored by PMSE

WEDNESDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 303

Biomaterials for Immunotherapy

H. Cheng, D. J. Irvine, *Organizers*

Z. Gu, *Organizer, Presiding*

H. Liu, J. Moon, *Presiding*

8:30 PMSE **523.** Phototherapy-triggered cancer immunotherapy with nanoparticles. **Z. Liu**

9:00 PMSE **524.** Nanotechnology-mediated delivery of nucleic acids for cancer therapy. **J. Shi**

9:30 PMSE **525.** Enhancing cancer immunotherapy using responsive biomaterials. **L. Tang**

10:00 PMSE **526.** Transiently thermosresponsive tetrahydropyran/furanylated -polyacrylamides: Synthesis, self-assembly, acid-triggered degradation and formulation of Amphotericin B as a vaccine adjuvant. B. De Geest, **S. Van Herck**

10:15 Intermission.

10:30 PMSE **527.** Modular nanostructures for immunotherapy. **C.A. Mirkin**

‡ *Cooperative Cosponsorship*

11:00 PMSE **528.** Nanolayer assembly as a platform for immunomodulatory release systems. **P.T. Hammond**

11:30 PMSE **529.** Ionic polyphosphazenes and their potential as immunotherapies. **A.K. Andrianov**

Section B

Moscone Center

Esplanade Ballroom 304

Polymers under Deformation

AFM & Nanoindentation Studies

Cosponsored by MPPG‡ and POLY‡

Financially supported by Asylum Research, ExxonMobil Chemical Company

A. I. Norman, *Organizer*

D. Yablon, *Organizer, Presiding*

8:30 PMSE **530.** Mechanical properties of polymers determined by nanoindentation. **A. Bushby**

9:00 PMSE **531.** Confined plasticity in polymer thin films. **G.L. Cross**, O. Brazil, J. de Silva, M. Chowdhury, W. Shi, W. Oliver, J.B. Pethica

9:30 PMSE **532.** Dynamic mechanical behavior of thermoset silica-filled rubber blends. **C. Dai**, Y. Chen, Y. Liu, J. Wang, F. Lo, C. Hsieh

10:00 Intermission.

10:10 PMSE **533.** AFM methods for aqueous probing of lubricious gel coatings for medical devices. **G.D. Haugstad**, M. Zeng, C. Colling, A. McCormick

10:40 PMSE **534.** Importance of the mechanical model used for the interpretation of atomic force microscopy measurements of the mechanical properties of nanofibers. **J. Hutter**, S. Makaremi, W. Wan

11:10 PMSE **535.** Pressing and sliding on gels and brushes. C.H. Mathis, R. Simic, L. Isa, **N.D. Spencer**

11:40 PMSE **536.** Deformation rate dependence of Atomic Force Microscope based nanomechanical measurements. **B. Pittenger**, J. He, L. Huang, T. Mueller, P. De Wolf

Section C

Moscone Center

Esplanade Ballroom 305

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

J. L. Almodovar, P. Byrley, *Presiding*

8:30 PMSE **537.** Epitaxial, ultra-thin gold coating as a barrier to prevent oxidation of silver nanowires. Y. Zhu, X. Ma, S. Kim, **P. Byrley**, M. Liu, R. Yan

8:50 PMSE **538.** Coordinate immobilization of Silver Nanoparticles on Aminated Polyethersulfone (AgNPs-APES) composite membrane for prolong and controlled silver ion (Ag^+) release. **M. Salman Haider**, G.N. Shao, K. Hee Taik

9:10 PMSE **539.** Bioinspired graphene-based nanocomposites via synergistic toughening. **Q. Cheng**

9:30 PMSE **540.** Nanohybrid films of functional biopolyimides with metal oxides by simple surface-engineering. **S. Dwivedi**, T. Kaneko

9:50 PMSE **541.** Multi-walled carbon nanotubes –Sulfur/High-Density Polyethylene (HDPE) multi-composites: Synthesis, crystallization, morphology and thermo-mechanical properties. K. Jena, **S. Al Hassan**

10:10 Intermission.

10:25 PMSE **542.** Engineering nanostructured hydroxyapatite/collagen composite scaffolds by green electrospinning. **J.L. Almodovar**, D. Castilla, M. Maldonado, P. Sundaram

10:45 PMSE **543.** Scalable manufacturing of biomimetic moldable hydrogels for industrial applications. **E.A. Appel**

11:05 PMSE **544.** Withdrawn.

11:25 PMSE **545.** CO2-selective composite membranes for pre-combustion carbon capture. **J. Bachman**, J.R. Long

11:45 PMSE **546.** Orthogonal oxime and Diels-Alder hyaluronan hydrogels as tunable matrices for multicellular tumour spheroid formation. **A.E. Baker**, R.Y. Tam, M.S. Shoichet

Section D

Moscone Center

Esplanade Ballroom 306

Innovations in Drug Delivery Systems & Combination Products

Novel Drug Delivery

A. S. Kulshrestha, *Organizer*

S. Sridharan, *Organizer, Presiding*

S. R. Raghavan, *Presiding*

8:30 PMSE **547.** Onion-like multilayered capsules based on stimuli-responsive polymers: A new design for multi-step release of drugs. **S.R. Raghavan**, B. Zarket

8:55 PMSE **548.** Electroresponsive drug delivery using conducting polymer nanoparticles. **D. Samanta**, N. Hosseini-Nassab, R.N. Zare

9:20 PMSE **549.** Multifunctional polyether-based lipids for liposomal nano drug carrier systems. **A. Danner**, H. Frey

9:45 PMSE **550.** Drug-eluting devices fabricated using the 3D printing technique Continuous Liquid Interface Production (CLIP) for controlled release applications. **C.J. Bloomquist**, R. Jansuziewicz, J.C. Luft, S.J. Mecham, A.Z. Wang, J.M. Desimone

10:10 Intermission.

10:20 PMSE **551.** Core cross-linked polypept(o)ide-based nanostructures: A novel platform for drug delivery. **K. Klinker**, T. Bauer, O. Schäfer, D. Huesmann, L. Braun, M. Barz

10:45 PMSE **552.** Optimizing drug release using silicone based implantable drug delivery systems. **N. Deorkar**

11:10 PMSE **553.** Magnetic nanostructures decorated hydrogels as a theranostic platform for biomedical applications. **V. Nandwana**, S. Ryoo, T.S. Zheng, M.M. You, V.P. Dravid

Section E

Moscone Center

Esplanade Ballroom 307

Synthesis, Processing & Device Engineering of Polymeric Electronic Materials

Financially supported by Tosoh, Japan Analytical Industry (JAI) Co., Ltd

C. Di, L. Fang, J. Mei, *Organizers*

C. Wang, *Presiding*

8:00 PMSE **554.** Controlling the active layer microstructure through conjugated block copolymers for solar cells and transistors. **E. Gomez**, B. Smith, M. Aplan, Y. Lee

8:30 PMSE **555.** Complementary semiconducting polymer blends melt-processed at 130°C for organic field-effect transistors with hole mobility approaching 1.0cm^2/Vs. **A. Gumyusenge**, X. Zhao, Y. Zhao, J. Mei

8:45 PMSE **556.** Withdrawn.

9:15 PMSE **557.** Inkjet printing high-resolution nanoparticle patterns by controlling substrate rheology. **M. Li**

9:35 PMSE **558.** Withdrawn.

9:55 Intermission.

10:15 PMSE **559.** Chemical blending vs physical blending: Comparing two approaches for polymer solar cells. Q. Zhang, M.A. Kelly, L. Yan, **W. You**

10:45 PMSE **560.** Surface-directed assembly for large-area coating of highly-aligned conjugated polymer thin films. **E. Mohammadi**, C. Zhao, Y. Meng, J. Mei, J. Zuo, D. Shukla, Y. Diao

11:00 PMSE **561.** Effect of chain length and comonomers/regiodefects on the stability of liquid crystalline phases in semiconducting polymers. **C.R. Snyder**

11:20 PMSE **562.** Interface engineering of graphene for enhanced photovoltaic performance. **Y. Wang**

11:40 PMSE **563.** Removable and recyclable conjugated polymers for highly selective and high-yield dispersion and release of low-cost carbon nanotubes. **T. Lei**, Z. Bao

Section F

Moscone Center

Esplanade Ballroom 308

Recent Advances in Multiblock Copolymers

Synthesis

Cosponsored by POLY

Financially supported by ExxonMobil Chemical Company, The Dow Chemical Company

Z. Bai, B. K. Long, J. Zhang, *Organizers*

C. Bates, *Presiding*

8:00 Introductory Remarks.

8:05 PMSE **564.** Sequence controlled block copolymers by RAFT polymerisation. **S. Perrier**

8:35 PMSE **565.** Design and synthesis of acrylate-based sulfonated superelastomers. **K. Misichronis**, W. Wang, Y. Wang, J.W. Mays, T. Saito, S. Cheng

9:05 PMSE **566.** Novel segmented Polyhydroxyurethane (PHU): Control of nanophase separation to achieve properties unlike and like those of segmented polyurethane and the potential to overcome challenges associated with recyclability of network PHU. **J.M. Torkelson**

9:35 Intermission.

9:55 PMSE **567.** Modifications to ethylene oxide /1,2-butylene oxide-based block copolymers and their effects on micellar behavior. **K. Harris**, E. Keene, V. Prasad

10:25 PMSE **568.** Complex ordered phases via designed multiblock copolymers. **A. Shi**

10:55 PMSE **569.** Architecture effects in block polymer self-assembly. **C. Bates**

11:25 PMSE **570.** Synthetic strategies for preparing (AB)n multiblock copolymers combining chain- and step-growth polymerization. **K.A. Cavicchi**

11:55 Concluding Remarks.

Section G

Moscone Center

Esplanade Ballroom 309

Molecular Engineering of Peptide Assembly

Peptides at Surface & Polypeptides

Financially supported by ACS Biomacromolecules

H. Cui, S. L. Perry, *Organizers*

A. Kros, M. V. Tirrell, *Organizers*, *Presiding*

8:15 PMSE **571.** Regulation and surface confinement of dynamic supramolecular peptide assemblies. **P. Besenius**, D. Spitzer, P. Ahlers, H. Frisch

8:45 PMSE **572.** Peptide-enhanced surface deposition of polymers and polymer nanoparticles. **H.A. Klok**

9:15 PMSE **573.** Designer synthetic polypeptides for cancer therapeutics. **P.T. Hammond**

9:45 Intermission.

10:00 PMSE **574.** Patterning and structure in polypeptide-based coacervates. **S.L. Perry**

10:30 PMSE **575.** Effect of surfaces and osmolytes in modulating peptide assembly. **J.E. Shea**

11:00 PMSE **576.** Synthesis of brush polypeptides. R. Baumgartner, H. Fu, Z. Song, Y. Lin, **J. Cheng**

11:30 PMSE **577.** Creating nanostructured films with high molecular weight periodically sequenced polypeptides. **R.S. Tu**

Bio-based Gels & Porous Materials

Biopolymer Hydrogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Polysaccharides: Practice & Applications

Novel Biocatalytic & Biopolymeric Approaches

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Innovative Chemistry & Materials for Electrochemical Energy Storage

Electrolytes & Interface

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Self-Healing Materials & Networks

Sponsored by POLY, Cosponsored by PMSE

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Polymerization, Coordination Chemistry & Interfacial Catalysis

Sponsored by INOR, Cosponsored by PMSE

WEDNESDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 303

Biomaterials for Immunotherapy

Z. Gu, D. J. Irvine, *Organizers*

H. Cheng, *Organizer, Presiding*

J. Shi, *Presiding*

1:30 PMSE **578.** Engineering silk-based microneedles for enhanced vaccines and cancer immunotherapy. **D.J. Irvine**

2:00 PMSE **579.** Designing biomateirals for CAR-T immunotherapy. **P. Wang**

2:30 PMSE **580.** Local delivery of checkpoints antibodies. **Z. Gu**, C. Wang, Y. Ye

Section B

Moscone Center

Esplanade Ballroom 304

Polymers under Deformation

Control of Deformation across the Length Scale for Advanced Polymer Materials

Cosponsored by MPPG‡ and POLY‡

Financially supported by Asylum Research, ExxonMobil Chemical Company

A. I. Norman, D. Yablon, *Organizers*

E. L. Heeley, Y. Yang, *Presiding*

1:30 PMSE **581.** Mechanical annealing and scraping of ferroelectric polymers at the nanoscale. **S. Hong**

2:00 PMSE **582.** Development of pressure-sensitive amorphous materials bearing TCAQ motifs. **Y. Ren**, S. Lee, J.M. Christensen, N. Plotnikov, M. Burgess, T.J. Martinez, D.D. Dlott, J.S. Moore

2:20 PMSE **583.** Determining the electromechanical response mechanism of nanostructured ionic block copolymers under an applied electric field. **B.S. Lokitz**, J. Dugger, M. Chen, T.E. Long, R. Kumar, J. Browning

2:40 PMSE **584.** Investigation into stress whitening production caused by coatings additives. **E. Radley**, C. Lowe, D. Gethin

3:00 Intermission.

3:10 PMSE **585.** Mechanochromic and photochromic fluorescence in epoxy. **R.E. Toivola**, S. Jang, D. Mannikko, S. Stoll, B. Flinn, A.K. Jen

3:30 PMSE **586.** Effect of uniformly applied force and molecular characteristics of a polymer chain on its adhesion to graphene and carbon nanotube substrates. **S. Pattanayek**

3:50 PMSE **587.** Omnidirectional nonlinear elasticity in liquid crystal elastomers. **A.D. Auguste**, N.P. Godman, T.J. White

4:10 PMSE **588.** Reliability of polymer backsheet structures in photovoltaic modules. **P. Yuen**, R. Dauskardt

Section C

Moscone Center

Esplanade Ballroom 305

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

E. Kynaston, *Presiding*

1:30 PMSE **589.** Effects of the temperature and UV intensity levels on degradation behaviors of high-density polyethylene. **J. Kim**, H. Hsueh, D.L. Hunston, D. Jacobs, L.N. Perry, C.C. White, L. Sung

1:50 PMSE **590.** Natural phenolic polymers for multi-functionalization of surface of fibers using laccase. **S. Kim**, H. Lee, J. Kim, F. Oliveira, J. Nakamatsu

2:10 PMSE **591.** Synthesis and characterization of cardanol based vinyl ester resins. **E. Kinaci**, E. Can, J.J. La Scala, G.R. Palmese

2:30 PMSE **592.** Tapping mode based AFM technique for quantitative characterization of mechanical properties of polymers. **M. Kocun**, A. Labuda, R. Proksch

2:50 PMSE **593.** Moldable photo-responsive elastomers from thermoreversible networks formed by triblock copolymer self-assembly. **Z. Kurji**, E. Bernhardt, M.G. Kuzyk, J.A. Kornfield

3:10 Intermission.

3:25 PMSE **594.** Patchy nanofibers from the self-assembly of a conjugated diblock copolymer. **E. Kynaston**, Y. Fang, J. Manion, N. Obhi, J. Howe, D.F. Perepichka, D.S. Seferos

3:45 PMSE **595.** Multi-scale coarse-graining with effective polarizabilities. **P.G. Lafond**, T.W. Sirk, J. Andzelm, S. Izvekov

4:05 PMSE **596.** Sulfonated Diels-Alder poly(phenylene) gas transport phenomena: Effect of chemistry and counterion. **T.D. Largier**, F. Huang, C.J. Cornelius

4:25 PMSE **597.** Temperature-dependent shape and morphology transformation of block copolymer particles by controlled assembly of thermoresponsive polymers. **J. Lee**, K. Ku, J. Shin, B. Kim

4:45 PMSE **598.** Design and synthesis of zwitterionic polyphosphoester-based coating materials for ^{64}Cu doped Au nanoclusters towards advanced *in vivo* pharmacokinetics. **R. Li**, G. Heo, L. Su, H. Wang, Y. Song, G. Sun, Y. Liu, K.L. Wooley

Section D

Moscone Center

Esplanade Ballroom 306

Innovations in Drug Delivery Systems & Combination Products

Biodegradable Vehicles for Drug Delivery

A. S. Kulshrestha, S. Sridharan, *Organizers*, *Presiding*

1:30 PMSE **599.** Development of a gemcitabine-polymer conjugate with enhanced cytotoxicity against a pancreatic cancer cell line. **F. Joubert**, S. Perrier, G. Pasparakis

1:55 PMSE **600.** Nitric oxide-releasing alginate as a biodegradable antibacterial scaffold. **M.R. Ahonen**, D.J. Suchyta, M. Schoenfisch

2:20 PMSE **601.** Polylactide-based multifunctional biodegradable polymer-drug conjugates. **H. Sun**, R. Zhang, W. Cheng, A. Commisso, M. Capeling, C. Cheng

2:45 Intermission.

2:55 PMSE **602.** Synthesis and self-assembly of amino functional AB-type biodegradable block copolymers. **F. Karagoez**, R. Dorresteijn, M. Klapper

3:20 PMSE **603.** Biodegradable, enzyme-responsive nanoparticles for acute myocardial infarction. **G.M. Policastro**, D. Wright, N.C. Gianneschi, K. Christman

3:45 PMSE **604.** Pro-Antimicrobial Networks with Degradable Acetals (PANDAs) prepared via thiol-ene photopolymerization. **D. Amato**, D.V. Amato, D.L. Patton

Section E

Moscone Center

Esplanade Ballroom 307

Synthesis, Processing & Device Engineering of Polymeric Electronic Materials

Financially supported by Tosoh, Japan Analytical Industry (JAI) Co., Ltd

C. Di, L. Fang, J. Mei, *Organizers*

Y. Diao, *Presiding*

1:30 PMSE **605.** Materials and measurements for flexible electronics. **D. DeLongchamp**

2:00 PMSE **606.** Mechanically adaptive electronic polymers for transparent self-healing artificial muscle. **C. Wang**

2:20 PMSE **607.** Mechanical properties of organic semiconductors for mechanically stable and intrinsically stretchable solar cells. **D.J. Lipomi**

2:50 PMSE **608.** Inducing elasticity through oligo-siloxane crosslinks for intrinsically stretchable semiconducting polymers. **G. Wang**, L. Shaw, J. Xu, T. Kurosawa, B.C. Schroeder, J. Oh, S.J. Benight, Z. Bao

3:05 PMSE **609.** Self-healable electrical insulation for high voltage aircraft. **T. Williams**, E. Shin, D. Scheiman, M. Lizcano, P. Mensah, J. Walker

3:20 Intermission.

3:40 PMSE **610. Award Address** (ACS Award for Team Innovation sponsored by ACS Corporation Associates). Development of photodefinable benzocyclobutene dielectric polymers: An enabling material for integrated circuit packaging. R. Devries, P. Garrou, **C.E. Mohler**, E. Moyer, T. Stokich

4:10 PMSE **611.** Highly stretchable polymer semiconductor films through nanoconfinement effect. **J. Xu**, S. Wang, Z. Bao

4:25 PMSE **612.** All-solution-processed stretchable transistor arrays based on polymer semiconductor and dielectric. **S. Wang**, F. Molina Lopez, J. Xu, J. Liu, J. Chung, Z. Bao

4:40 PMSE **613.** Effects of sterilization on self-softening thiol-ene/acrylate polymers for bioelectronics. **M. Ecker**, V. Danda, J. Pancrazio, W. Voit

Section F

Moscone Center

Esplanade Ballroom 308

Recent Advances in Multiblock Copolymers

Characterization

Cosponsored by POLY

Financially supported by ExxonMobil Chemical Company, The Dow Chemical Company

B. K. Long, J. Zhang, *Organizers*

Z. Bai, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 PMSE **614.** Control of gelation and syneresis of aqueous cellulosic ether materials. **R.L. Sammler**, C.E. Mohler, R. Adden, M. Brackhagen, J.D. Moore, B. Huebner-Keese

1:35 PMSE **615.** Thermoplastic elastomers from linear and star polymers containing polyethylene blocks. **R.A. Register**, A.B. Burns

2:05 PMSE **616.** Bicontinuous morphologies from binary blends of narrow dispersity block polymers. **M.K. Mahanthappa**

2:35 PMSE **617.** Dynamic properties of polyolefin block copolymers prepared through living coordination polymerization. **L.R. Sita**

3:05 Intermission.

3:25 PMSE **618.** Strain hardening in immiscible PE/PP blends via interfacial reinforcement with PE-cb-PP comb-block copolymers. **C. Lopez-Barron**, A.H. Tsou, P. Jiang, D.J. Crowther

3:55 PMSE **619.** Using crystallisation driven assembly to prepare 2-dimensional nanomaterials. **R.K. OReilly**

4:25 PMSE **620.** Structure, phase behavior, and rheology of block copolymers in crosslinkable acrylate monomers. **Z. Bai**, J. Huang, V. Ginzburg, M. Williams, K. Penkala, J. Joo, C. Taylor, L. Chen, C.J. Tucker

4:55 Concluding Remarks.

Section G

Moscone Center

Esplanade Ballroom 309

Molecular Engineering of Peptide Assembly

Peptides for Medicine

Financially supported by ACS Biomacromolecules

A. Kros, M. V. Tirrell, *Organizers*

H. Cui, S. L. Perry, *Organizers*, *Presiding*

1:30 PMSE **621.** Supramolecular polypeptide materials for modulating immune and inflammatory processes. **J. Collier**

2:00 PMSE **622.** Tit for tat: Design evolution of anticancer peptides from self-assembled hydrogels and how cancer cells gain resistance to their action. **J.P. Schneider**

2:30 PMSE **623.** Self-assembling multidomain peptides for tissue regeneration. **J.D. Hartgerink**

3:00 Intermission.

3:15 PMSE **624.** Designable peptide assemblies. **V.P. Conticello**

3:45 PMSE **625.** Designing peptides for use in regenerative medicine and biosensing. **M. Stevens**

‡*Cooperative Cosponsorship*

4:15 PMSE **626.** Peptide-polymer and asymmetric peptide assemblies. **S.I. Stupp**, L.C. Palmer, Z. Yu

4:45 PMSE **627.** Engineering peptide hydrogels: From fibres to networks. A.F. Miller, **A. Saiani**

5:15 Concluding Remarks.

Bio-based Gels & Porous Materials

Biopolymer Organogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Polysaccharides: Practice & Applications

Novel Materials & Methodologies

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Innovative Chemistry & Materials for Electrochemical Energy Storage

Anode Materials & Li-S

Sponsored by ENFL, Cosponsored by MPPG² and PMSE

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Biomaterials

Sponsored by POLY, Cosponsored by PMSE

ACS Award in Polymer Chemistry: Symposium in honor of Murugappan Muthukumar

Sponsored by POLY, Cosponsored by PMSE

2017 Priestley Medalist: Symposium in honor of Tobin J. Marks

Catalysis: Characterization, Computations & Reactivity

Sponsored by INOR, Cosponsored by PMSE

WEDNESDAY EVENING

POLY/PMSE Plenary Lecture & Awards

Sponsored by POLY, Cosponsored by PMSE

THURSDAY MORNING

Section A

Moscone Center

Esplanade Ballroom 303

Biomaterials for Immunotherapy

H. Cheng, Z. Gu, D. J. Irvine, *Organizers*

E. A. Scott, L. Tang, Y. Yu, *Presiding*

8:30 PMSE **628.** Functionalized polymersomes as carriers for immune activation. **R.W. Zentel**, S. Schuerer, R. Krini, M. Scherer, M. Helm, M. Bros, R. Ose, H. Jonuleit

8:45 PMSE **629.** Immune-modulator polymersomes. **A. Poma**, C. Lopez Vasquez, L. Rizzello, Y. Zhu, D. Cecchin, J. Gaitzsch, I. Romano, E. Mele, C.K. Williams, G. Battaglia

9:00 PMSE **630.** Rationalization of a lipid-polymeric nanoparticle-based nicotine nanovaccine for immunotherapy against nicotine addiction: A focus on hapten localization. **Z. Zhao**, T. Harmon, P. Pentel, C. Zhang

9:15 PMSE **631.** Engineering anti-cancer immunity using polymeric nanoparticles that transform into synthetic cell surface receptors in response to intracellular pH. B. De Geest, **R. De Coen**

9:30 PMSE **632.** Enhanced cancer immunotherapy by microneedle patch-assisted delivery of anti-PD1 antibody. Z. Gu, **C. Wang**, Y. Ye

9:45 Intermission.

10:00 PMSE **633.** Synthetic polymers delivering peptide neoantigens and TLR-7/8 agonists as personalized cancer vaccines. **G. Lynn**, C. Sedlik, R. Laga, O. Lantz, R. Seder

10:15 PMSE **634.** Tunable glycopolypeptides bearing pattern-recognition motifs affect phagocytosis and cytokine expression. **J. Kramer**, M. Zhou, C. Delaveris, C.R. Bertozzi

10:30 PMSE **635.** Polypept(o)ide based tumor immune therapy: Combining vaccination and abolishment of immune tolerance. **M. Barz**

10:45 PMSE **636.** Intracellular unfolding nanoparticles for the delivery of immune-stimulatory cues towards anticancer immunity. **L. Nuhn**, B. De Geest

Section B

Moscone Center

Esplanade Ballroom 304

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

R. Y. Tam, H. Wang, *Presiding*

8:30 PMSE **637.** Stimuli-responsive hyaluronan-based hydrogels provide biochemically-defined, biomimetic scaffolds for 3D cell culture. **R.Y. Tam**, S. Fisher, A.E. Baker, L. Smith, L. Julian, J. Yockell-Lelievre, W. Stanford, M.S. Shoichet

8:50 PMSE **638.** Effect of branching chain parameter on rheological behavior of comb-like (co)polymers with high branching degree. **T. Tang**

9:10 PMSE **639.** Effects of pendant alkyl chain length on water barrier properties of epoxy/amine thermosets. **J. Vergara**, G.R. Palmese

9:30 PMSE **640.** Toughening hybrid nanocomposites with molecularly confined polymers by chemically tuning the polymer-surface interaction. **C. Wang**, S.G. Isaacson, K. Lionti, W. Volksen, T.P. Magbitang, R. Dauskardt, G. Dubois

9:50 Intermission.

10:05 PMSE **641.** Novel polyamide liquid core-shell microcapsules responsive to solvent environments. **H. Wang**, S.C. Zimmerman, J.M. Grolman, J. Moore

10:25 PMSE **642.** Architectural effect of organic nanoparticles on block copolymer thin film orientation. **H. Wang**, S. Kim, A. Khan, J. Huh, J. Bang

10:45 PMSE **643.** Air-triggered self-sealing polymeric materials spontaneously formed at liquid/air interface. **Y. Wang**, H. Lee

11:05 PMSE **644.** Smart microgels as functional valves for detection of Pb^{2+}. **Y. Wang**, Z. Liu, H. Peng, L. Zhang, W. Wang, X. Ju, R. Xie, L. Chu

11:25 PMSE **645.** Polymeric exfoliating dispersants of poly(oxyethylene)-imide-amide structures for waterborne delaminating graphite into graphene and uses in electrostatic-heat dissipation and flexible conductive films. **G. Wang**, **S. Shen**, W. Wang, W. Lo, C. Ho, Y. Wang, J. Lin

Section C

Moscone Center

Esplanade Ballroom 305

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

M. J. Worthington, K. Yang, *Presiding*

8:30 PMSE **646.** Formation of well-defined, functional nanotubes via osmotically induced shape transformation of biodegradable polymersomes. **D.S. Williams**, L.K. Abdelmohsen, D.A. Wilson, J. van Hest

8:50 PMSE **647.** Heterogeneous nucleation of lamella polypropylene on SWNT-alumina hybrid platelets for discontinuous composite reinforcement. **G. Winter**, J. Faust, M. Minus

9:10 PMSE **648.** Renewable polysulfides for mercury capture and environmental remediation. **M.J. Worthington**, J.M. Chalker

9:30 PMSE **649.** Producing low reflectance coatings utilizing synergistic effects of polymer phase separation. S.L. Giles, N.W. Heller, C.R. Clayton, **J.H. Wynne**

9:50 Intermission.

10:05 PMSE **650.** Withdrawn.

10:25 PMSE **651.** Combined material and photochemical printing with cantilever-free polymer tip arrays. **Z. Xie**, C.A. Mirkin

10:45 PMSE **652.** Environmentally friendly high-performance furan-based polyimides. **S. Yadav**, J.J. La Scala, J.M. Sadler, G.R. Yandek, G.R. Palmese

11:05 PMSE **653.** Withdrawn.

11:25 PMSE **654.** Diels-Alder rapid extrusion 3D printing of melt-processable thermoset polymers. **K. Yang**, J. Grant, W. Archer, W. Voit

Section D

Moscone Center

Esplanade Ballroom 306

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

I. Yilgor, L. Zou, *Presiding*

8:30 PMSE **655.** Stiffer but more healable exponential layered assemblies with boron nitride nanoplatelets. **M. Yang**

8:50 PMSE **656.** Hydrolysable polyureas based on hindered urea bonds. **Y. Yang**, H. Ying, J. Cheng

9:10 PMSE **657.** Chemistry in porous polymers: Fine tuning chemical interactions. **C.T. Yavuz**, V. Rozyyev, Y. Song, N.A. Dogan, Y. Hong

9:30 PMSE **658.** Fabrication of microporous PLA foams via thermally induced phase separation and solvent exchange. **I. Yilgor**, E. Yilgor, O.C. Onder

9:50 Intermission.

10:05 PMSE **659.** 3D printed bioceramic/biodegradable polymer scaffolds for bone tissue engineering. **J. Yu**, Y. Xu, S. Li, G.V. Seifert, M. Becker

10:25 PMSE **660.** One-pot synthesis of inorganic nanoparticle vesicles via surface-initiated polymerization-induced self-assembly. **Y. Zheng**, Y. Huang, Z. Abbas, B.C. Benicewicz

10:45 PMSE **661.** Design and synthesis of amine-functionalized Porous Polymer Networks (PPNs) for carbon capture. **L. Zou**, H. Zhou

11:05 PMSE **662.** Utilizing hard transparent arrays for polymer pen lithography for high resolution patterning. **J. Hedrick**, K.A. Brown, E.J. Kluender, M. Cabezas, P. Chen, C.A. Mirkin

11:25 PMSE **663.** Enhanced piezoelectric response of electrospun PVDF with ZnO nanorods. **M. Kim**, J. Fan, Y. Wu

Section E

Moscone Center

Esplanade Ballroom 307

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

M. Graffeo, P. Samanta, *Presiding*

8:30 PMSE **664.** Dynamic hydrogels with tunable mechanics and their biological applications. **J. Lou**, F. Liu, Y. Xia

8:50 PMSE **665.** Fatigue of injection molded and 3D-printed polycarbonate urethane in solution. **A. Miller**, D.L. Safranski, K.E. Smith, D.G. Sycks, R.E. Guldberg, K. Gall

9:10 PMSE **666.** Homogenous nucleated crystallization of poly (ethylene oxide) under confinement in electrospun nanofibers of polystyrene/poly(ethylene oxide) blends. **P. Samanta**

9:30 PMSE **667.** Rheological characteristics of hairy particles in oscillatory shear flow. **W. Xiong**, S. Li, X. Wang

9:50 Intermission.

10:05 PMSE **668.** Kirigami nanocomposite as strain-tunable diffraction gratings. **L. Xu**, N. Kotov

10:25 PMSE **669.** Synthesis and properties of quanternized polyethersulfones and their applications as alkaline anion exchange. **J. Chen**, P. Chen, H. Chen

10:45 PMSE **670.** Ion transport and nanoscale morphology in cyclopropenium-based polymerized ionic liquids. **J. Freyer**

11:05 PMSE **671.** Drug delivery: Accelerating the drug development pathway for increased speed to patient. **M. Graffeo**

11:25 PMSE **672.** Single particle fluorescence microscopy reveals unexpected photobrightening in dye aggregates. **D. Hinton**, J. Ng, R.H. Goldsmith

Section F

Moscone Center

Esplanade Ballroom 308

Recent Advances in Multiblock Copolymers

Application

Cosponsored by POLY

Financially supported by ExxonMobil Chemical Company, The Dow Chemical Company

Z. Bai, B. K. Long, J. Zhang, *Organizers*

A. Lane, *Presiding*

8:00 Introductory Remarks.

8:05 PMSE **673.** Block copolymer-directed assembly of pharmaceutical nanoparticles: Effects of Mw and chemistry on assembly, delivery, and in vivo performance. R.F. Pagels, H. Lu, B.K. Wilson, S.M. D'Addio, S.M. Ansell, L.D. Mayer, C. Vauthier, A. Pietrangelo, A. Panagiotopoulos, **R.K. Prudhomme**

8:35 PMSE **674.** Janus composites and interfacial engineering. **Z. Yang**

9:05 PMSE **675.** Orientation control in thin films of a high-χ block copolymer with a surface active embedded neutral layer. **J. Zhang**, P.D. Hustad, P. Trefonas

9:35 PMSE **676.** Polypropylene-based olefin block copolymers as compatibilizers for polyethylene and polypropylene. **Y. Hu**

10:05 Intermission.

10:25 PMSE **677.** Multiblock copolymer phase separation in thermoset polyurethanes. **K. Aou**

10:55 PMSE **678.** Strengthening thermosensitive ABC linear triblock copolymer micellar hydrogels with thermosensitive hairy nanoparticles. **B. Zhao**

11:25 PMSE **679.** Aligned 5 nm block copolymer lamellae for high resolution lithography applications. **A. Lane**, X. Yang, M.J. Maher, G. Blachut, Y. Asano, Y. Someya, S. Sirard, A. Mallavarapu, C.J. Ellison, C.G. Willson

11:55 PMSE **680.** Bioorthogonal synthesis of protein mimetic multiblock copolymers. **X. Jia**

12:25 Concluding Remarks.

Section G

Moscone Center

Esplanade Ballroom 309

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

T. Hussain, C. Zhu, *Presiding*

8:30 PMSE **681.** Fabrication highly conductive copper powder and films by chemical methods with polymer dispersant. **P. Huang**, J. Lin, Y. Leu

8:50 PMSE **682.** Establishment of correlation between MWCNTs dimensions and electrical character of MWCNTs based polymer composites. **T. Hussain**, A. Alvi, A. Mujahid

9:10 PMSE **683.** Production of core-sheath structured nanofibrous membranes for high temperature fuel cells. **S. Jahangiri**, I. Aravi, Y.Z. Menceloglu, L. Isikel Sanli, E. Ozden Yenigun

9:30 PMSE **684.** Crystalline MoOx thin-films as hole transport layer in organic solar cells. A. Cauduro, R. dos Reis, M. Ahmadpour, G. Chen, A. Schmid, C. Méthivier, N. Witkowski, H. Rubahn, **M. Madsen**

9:50 Intermission.

10:05 PMSE **685.** Uniformly distributed heteroatoms containing two-dimensional networks. **J. Mahmood**, J. Baek

10:25 PMSE **686.** Role of enhanced hydrogen bonding of selectively reduced graphite oxide in fabrication of poly(vinyl alcohol) nanocomposites in water as EMI shielding material. **K. Manna**

10:45 PMSE **687.** Anti-icing property of transparent heater with super-repellency and electrothermogenesis exhibited by PEDOT:PSS/cyanoacrylate composite nanoparticles. **S. Shiratori**, T. Matsubayashi, M. Tenjimbayashi

11:05 PMSE **688.** Host-guest self-assembled surface with controllable switch for bacteria killing and detaching. **Z. Shi**, W. Zhao

11:25 PMSE **689.** Conformational control of π-conjugated molecules using hydrogen bonds. **C. Zhu**, A. Mu, Z. Guo, L. Fang

Bio-based Gels & Porous Materials

Aero-, Cryo- & Xerogels

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Polysaccharides: Practice & Applications

New Functional Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

Innovative Chemistry & Materials for Electrochemical Energy Storage

Electrochemical Catalysis & Energy Conversion

Sponsored by ENFL, Cosponsored by MPPG‡ and PMSE

Smart Polymeric Materials from Cyclodextrins: Novel Designs & Applications

Stimuli-Responsive Polymers & Polymer Processing

Sponsored by POLY, Cosponsored by PMSE

THURSDAY AFTERNOON

Section A

Moscone Center

Esplanade Ballroom 303

General Papers/New Concepts in Polymeric Materials

M. Grunlan, *Organizer*

R. C. Steinhardt, S. A. Sydlik, *Presiding*

1:30 PMSE **690.** Improvement in dynamic mechanical and barrier properties of innovative polymer clay nanocomposites based on polystyrene matrix. **I. Soltani**, R.J. Spontak

1:50 PMSE **691.** Effect of fatty acid chain length in amidoamine crosslinkers on material properties of epoxy systems. **A. Sridhar**, J. Vergara, C. Abrams, G.R. Palmese

2:10 PMSE **692.** Facile *in-situ* polymer brush characterization using whispering gallery mode sensors. **A. Stanton**, R.C. Bailey

2:30 PMSE **693.** Discovering the cellular origin of agonist synergies towards the development of better vaccines. **R.C. Steinhardt**, B. Moser, A. Esser-Kahn

2:50 Intermission.

3:05 PMSE **694.** Efficient dispersion of mineral hemostatics in a poly-HIPE scaffold for severe wound treatment. **B. Streifel**, J. Lundin, C.L. McGann, J.H. Wynne

3:25 PMSE **695.** Functional triblock bottlebrush polymers: From synthesis toward biomedical applications. **L. Su**, G. Sun, K.L. Wooley

3:45 PMSE **696.** Polymer complexation and the beautiful lie: Complex laddering of globular structures. **T. Swift**, S. Rimmer

4:05 PMSE **697.** Polyphosphate and polyamide modified graphite as a degradable, cell instructive scaffold for bone regeneration. **S.A. Sydlik**, A. Arnold, B. Holt

4:25 PMSE **698.** Investigating dynamic mechanical properties of inventive polyvinylacetate clay nanocomposites with improved gas barrier properties. **I. Soltani**, R.J. Spontak

Bio-based Gels & Porous Materials

Open-Porous Carbon Materials

Sponsored by CELL, Cosponsored by AGFD, CARB, COLL, PMSE and POLY

Advances in Polysaccharides: Practice & Applications

Preparation, Characterization & Applications

Sponsored by CELL, Cosponsored by AGFD, CARB, MPPG‡, PMSE and POLY

PROF

Division of Professional Relations

R. Libby, *Program Chair*

SOCIAL EVENTS:
Reception, 5:00 PM: Tue

BUSINESS MEETINGS:
Business Meeting, 3:00 PM: Tue

SUNDAY MORNING

Section A

Hotel Nikko San Francisco

Nikko Ballroom III

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Financially supported by Peter K. Dorhout (ACS President-Elect) & Merck

M. Morris, J. S. Nowick, *Organizers*

P. Rodenbough, *Presiding*

9:00 Introductory Remarks.

9:05 PROF **1.** Coupling multiple proton transfers to electron transfer in bio-inspired Tyr-His models. **M.T. Huynh**, S.J. Mora, M. Villalba, A. Teillout, J.D. Gust, T.A. Moore, A.L. Moore, S. Hammes-Schiffer

9:25 PROF **2.** Ligand to metal charge transfer in early transition metal bicyclic guanidinate complexes. **J. Olson**, D. Swenson, L. Messerle

9:45 PROF **3.** New materials from superatomic build blocks: The $Fe_8O_4pz_{12}Cl_4$ cluster as a probe for singlet fission and novel battery materials. **A. Pinkard**, M. Trinh, A. Pun, S. Sanders, E. Kumarasamy, M. Sfeir, L. Campos, X. Roy, Z. Xiaoyang

10:05 PROF **4.** In situ Raman investigation of chemical vapor deposition of WN_xC_y thin films from tungsten imido precursors. **M. Nolan**, A. Koley, S. Kim, T.J. Anderson, L. McElwee-White

10:25 Intermission.

10:40 PROF **5.** Direct observation of localized surface plasmon resonances in single nanocrystals of doped metal oxides. **R.W. Johns**, D.J. Milliron

11:00 PROF **6.** Theoretical and numerical study of catalytic metal-noble metal nanoparticle aggregates for plasmon-mediated catalysis. **N.P. Montoni**, D.J. Masiello

11:20 PROF **7.** Soft donor coordination compounds of the mid to late actinides. **S.S. Galley**, T.E. Albrecht-Schmitt

11:40 PROF **8.** Investigation of f-element bonding with neutral soft chalcogen donors for lanthanide/actinide separations. **A.V. Blake**, S.R. Daly

SUNDAY AFTERNOON

Section A

Hotel Nikko San Francisco

Nikko Ballroom III

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Financially supported by Peter K. Dorhout (ACS President-Elect) & Merck

M. Morris, J. S. Nowick, *Organizers*

M. Nolan, *Presiding*

1:40 Introductory Remarks.

1:45 PROF **9.** Development of a unified strategy for the syntheis of enmein-type *ent*-kauranoids. **J.C. Beck**, S.E. Reisman

2:05 PROF **10.** Chiral phosphoric acids as Brønsted acid promoters of latent nucleophile reactions. **R.A. Escobar**, S. Schaus

2:25 PROF **11.** Withdrawn.

2:45 PROF **12.** Spin-Selective generation of triplet nitrenes: Olefin aziridination through visible-light photosensitization of azidoformates. **S. Scholz**, E. Farney, S. Kim, D. Bates, T.P. Yoon

3:05 Intermission.

3:20 PROF **13.** Aldol condensation of biomass-derived feedstocks in HZSM-5 zeolite: Quantum chemistry and experiments point to keto/enol as the rate-determining step. **A.N. Migues**, Q. Sun, S. Vaitheeswaran, W. Sherman, X. Qi, W. Fan, S.M. Auerbach

3:40 PROF **14.** Automated reaction progress analysis: A rapid and robust method for elucidating catalyst monopoly. **R. Chung**, J. Hein

4:00 PROF **15.** Panel discussion. Celebrating LGBT identities in chemistry: Opportunities, challenges, and perspectives. **M. Morris**, **J.S. Nowick**

‡*Cooperative Cosponsorship*

Chemical Angel Network: Chemists Investing in Chemical Companies

Sponsored by BMGT, Cosponsored by PROF‡ and SCHB‡

Holy Grails in Chemistry: Celebrating the 50th Anniversary of Accounts of Chemical Research Journal

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CATL, CELL, COLL, ENVR, HIST, I&EC, MEDI, MPPG‡, ORGN and PROF

Starting a Successful Research Program at a PUI

Sponsored by YCC, Cosponsored by PROF

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Sponsored by WCC, Cosponsored by CHED, CMA and PROF

SUNDAY EVENING

Section A

Moscone Center

Exposition, Halls B/C

General Posters

R. Libby, *Organizer*

6:30 - 8:30

PROF **16.** White light from hybrid water soluble Au (I) phosphor systems for OLED applications. **C. Williams**, E.N. Benton, S.B. Marpu, M.A. Omary

PROF **17.** Collaborations and outreach: A review of ACS presence at the 2017 Out to Innovate™ career summit for LGBTQ+ people in STEM. **B.L. Belmont**, C.J. Bannochie

PROF **18.** Materials for teaching professionalism in chemistry. **S.M. Schelble**

Entrepreneurial Opportunities in Chemistry

Sponsored by YCC, Cosponsored by BMGT, PROF and SCHB

MONDAY MORNING

Section A

Hotel Nikko San Francisco

Nikko Ballroom III

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Financially supported by Peter K. Dorhout (ACS President-Elect) & Merck

M. Morris, J. S. Nowick, *Organizers*

A. Mercer, *Presiding*

9:00 Introductory Remarks.

9:05 PROF **19.** Understanding the unusual isotope effects in ozone formation for applications to atmospheric chemistry and climate. **A.H. Kazez**, K.A. Boering

9:25 PROF **20.** Fulvenallene and fulvenallenyl photodissociation dynamics at 248 nm. **M. Shapero**, I.A. Ramphal, D.M. Neumark

9:45 PROF **21.** Irradiation of secondary organic aerosol material in the presence of volatile organic compounds: The role of photosensitization. **K.T. Malecha**, S.A. Nizkorodov

10:05 PROF **22.** Chemical x-ray photodiffraction for structural characterization of short-lived intermediates. **P.P. Rodenbough**, P. Naumov

10:25 Intermission.

10:40 PROF **23.** Megasupramolecules as molecular probes of turbulence. **R. Lhota**, R. McMullen, D. Huynh, M. Wei, J.A. Kornfield, B. McKeon

11:00 PROF **24.** Effect of annealing temperature on graphene supported nickel catalysts with regards to its structure and urea oxidation properties. **D. Glass**, S.G. Prakash, G. Olah

11:20 PROF **25.** Dietary proanthocyanidin detector response factors have appreciable variability. **M.R. Dorris**, B.W. Bolling

Space Chemistry: How it Helps Space Exploration

Sponsored by YCC, Cosponsored by CPRC and PROF

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC, PRES‡ and PROF

Celebrating 90 years of the WCC: Reflections of Past Chairs

Sponsored by WCC, Cosponsored by PRES and PROF

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Section A

Hotel Nikko San Francisco

Nikko Ballroom III

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

Financially supported by Peter K. Dorhout (ACS President-Elect) & Merck

M. Morris, J. S. Nowick, *Organizers*

R. Lhota, *Presiding*

2:00 Introductory Remarks.

2:05 PROF **26.** Advancing ferrocenyl derivatives pharmacophores throughout the incorporation of heterocycles in their scaffolds. **J.C. Aponte-Santini**, I. Montes-González, J. Davila, D.J. Sanabria Rios, Y. Morales-Lozada, A. Baerga-Ortiz, A.R. Guadalupe Quinones, A. Serrano-Brizuela, E. Colón-Lorenzo, F.T. Halaweish

2:25 PROF **27.** Development of a selective and stable anti-cancer agent by exploiting high levels of reactive oxygen species. **K.G. Earnest**, A.L. Kadekaro, Y. Zhang, E.J. Merino

2:45 PROF **28.** Thioether-bridged peptide macrocycles as inhibitors of the Sonic Hedgehog/patched 1 protein-protein interaction. **A. Owens**, R. Fasan

3:05 PROF **29.** Enzyme-Directed imidazoquinolines for cancer immunotherapy. **J. Hantho**, R.J. Mancini, A.E. Nielsen

3:25 Intermission.

3:40 PROF **30.** Engineering a synthetic peptide/GPCR communication language in yeast. **J. Brisbois**, S. Billerbeck, M. Jimenez, N. Agmon, M. Shen, J. Temple, J. Boeke, V.W. Cornish

4:00 PROF **31.** Backbone C5 hydrogen bonds in proteins. **R.W. Newberry**, R.T. Raines

4:20 PROF **32.** Withdrawn.

4:40 PROF **33.** Student accuracy and confidence on items assessing problematic topics in the biochemistry sequence. **A. Mercer**, A. Wolfson, J.E. Lewis

Rising Star Award Symposium

Sponsored by WCC, Cosponsored by BIOL, ENFL and PROF

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Space Chemistry: How it Helps Space Exploration

Sponsored by YCC, Cosponsored by CPRC and PROF

Teaching, Researching & Community Building in the Global Chemical Enterprise

Sponsored by IAC, Cosponsored by BMGT‡, ENVR‡, I&EC‡, PRES‡ and PROF‡

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY EVENING

Section A

Moscone Center

Hall D

Sci-Mix

R. Libby, *Organizer*

8:00 - 10:00

16-18. See previous listings.

TUESDAY MORNING

Section A

Hotel Nikko San Francisco

Monterey I

Producing Knowledgeable, Well-Rounded, T-Shaped Chemists for the 21st Century: Current Perspectives from High School, Undergraduate & Graduate Educators

Cosponsored by BMGT, CHED and PRES

J. L. Bryant, J. C. Giordan, *Organizers*

S. M. Graham, *Organizer, Presiding*

8:40 PROF **34.** Depth and breadth. Content and skills. Experts and generalists. The emerging need for T-shaped individuals: Opening overview. **S.M. Graham**

8:50 PROF **35.** Preparing T-shaped chemists: Using big ideas to understand and communicate chemistry. **G.T. Rushton**

9:10 PROF **36.** Process - The missing element. **D. Hanson**

9:30 PROF **37.** Transformational and innovative approaches to STEM graduate education – building T shaped professionals with a Lens of the Market® as well as a Lens of Science. J.C. Giordan, M. Dolgos, M. Storksdieck, **R.G. Carter**

9:50 Intermission.

10:00 PROF **38.** Remembering to cross your t: Teaching and learning chemistry with today's teenagers. **J.L. Ball**

10:20 PROF **39.** Who gives a darn? An application based organic chemistry curriculum to develop T-shaped students. **E.C. Bucholtz**

10:40 PROF **40.** Transformational and innovative approaches to STEM graduate education: Building T shaped professionals with real world internship experiences. **S.E. York**

11:00 Intermission.

11:10 Interactive Panel With Facilitated Q&A.

11:30 Concluding Remarks.

11:40 "Office Hours" with Speakers

Chemists & Writing for Fun & Profit: Write Your Own Career

Sponsored by SCHB, Cosponsored by CPRC and PROF

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Sponsored by WCC, Cosponsored by CHED, CMA and PROF

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Materials Chemistry of Solutions & Solids for a Sustainable Future

Sponsored by INOR, Cosponsored by BMGT‡, MPPG and PROF‡

Advancing Undergraduate Research

Research Supportive Curricular Innovations

Sponsored by CHED, Cosponsored by PROF

TUESDAY AFTERNOON

Section A

Hotel Nikko San Francisco
Monterey I

REU Chemistry in Action: Student Perspectives

L. M. Watkins, *Organizer*

S. A. France, *Presiding*

1:30 Introductory Remarks.

1:35 PROF **41.** Synthetic studies of redox-active, self-associating macrocycles: Perspectives on a materials chemistry REU. **R.E. Fadler**, J. Dobscha, H.D. Castillo, S.L. Tait, A.H. Flood

1:55 PROF **42.** Passport to success: Research experience abroad. **S. Ramirez**

2:15 PROF **43.** Understanding the products of the bisulfite reaction with 5-methylcytidine and 5-hydroxymethyl-2'-deoxycytidine. **H. Donelick**, A.M. Fleming, C.J. Burrows

2:35 PROF **44.** Synthesis of a new mixed occupancy $Yb_{14-x}Ca_xMgSb_{11}$ (x = 0,1,2) for thermoelectric device application. **K. Meyer**, S. Kauzlarich, E.L. Kunz Wille

2:55 Intermission.

3:10 PROF **45.** Aspect ratio dependent growth mechanism revealed in gold nanorod synthesis. **T. Ripplinger**, J. Zhao, S. Thota

3:30 PROF **46.** Correlation between Hammett parameters and vibrational Stark effects in benzonitrile derivatives. **J. Alvarez Duque**, J.R. Hunt, J. Dawlaty

3:50 PROF **47.** Intracellular tracing of deferasirox and its Ti(IV) complex by the FITC probe to study their cytotoxic mechanism of action. **M. Kowaleff**, Y. Delgado, A.D. Tinoco, Z. Torres, A.M. Vázquez

4:10 PROF **48.** Antibiotic-carbon dot conjugate for imaging and as bactericidal agents. **I. Sun**, I.V. Ogungbe

4:30 Concluding Remarks.

Entrepreneurship in Biotechnology, Advanced Materials, Drug Discovery & Information Systems

Sponsored by SCHB, Cosponsored by MEDI and PROF

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

ACS Award in the Chemistry of Materials: Symposium in honor of Douglas A. Keszler

Chemists Leading the Charge: Chemists Using Business Acumen & Transformative Research to Address Societal Needs

Sponsored by INOR, Cosponsored by BMGT‡, MPPG, PRES and PROF‡

Advancing Undergraduate Research

Focus on Early Access to Research & Broadening Participation of Underrepresented Groups

Sponsored by CHED, Cosponsored by CMA‡, PROF‡ and WCC

TUESDAY EVENING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY MORNING

Section A

Hotel Nikko San Francisco
Monterey I

Looking Beyond Your Current Boundaries: What's the Next Step?

Academic Route: PhD to Postdoc to Ass. Prof.

Cosponsored by BMGT and YCC

M. Grandbois, *Organizer*

J. T. Kelly, *Organizer, Presiding*

9:00 Introductory Remarks.

9:05 PROF **49.** Crossing boarders as a postdoc: An unexpected journey after a PhD. **J.T. Kelly**

9:35 PROF **50.** Securing a tenure-track position at a research university: The hiring process. **N. Hammer**

10:05 PROF **51.** Professor Gig at a medium-sized PUI. **R.C. Fortenberry**

10:35 Intermission.

10:45 PROF **52.** Expanding the academic excellence model through gender diversity. **D. Stallings**, S. Iyer, R. Hernandez

11:15 PROF **53.** Creating a mentoring culture to improve demographic diversity in academia. **S. Iyer**, D. Stallings, R. Hernandez

11:45 Concluding Remarks.

Advancing Undergraduate Research

Sponsored by CHED, Cosponsored by CMA, PROF and WCC

WEDNESDAY AFTERNOON

Section A

Hotel Nikko San Francisco
Monterey I

Looking Beyond Your Current Boundaries: What's the Next Step?

Industrial Route: PhD, Postdoc, Scientist

Cosponsored by BMGT and YCC

J. T. Kelly, *Organizer*

M. Grandbois, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 PROF **54.** Thinking about a career in industry? **C.J. Murphy**

2:05 PROF **55.** Realizing you're ready: How my everyday experience translated into job seeking success. **S.L. Hemmingson**

2:35 PROF **56.** Personal brand development and social networking strategies for professional chemists. **J.L. Maclachlan**

3:05 Intermission.

3:15 PROF **57.** Managing your career with power! How to get that first promotion and prepare yourself for future roles. **M. Grandbois**, S. Collick

3:45 PROF **58.** Career transitions for a young industrial chemist: From the bench to management. **A.K. Gupta**, M. Grandbois

4:15 Concluding Remarks.

RUBB

Rubber Division

W. Stahl, *Program Chair*

MONDAY EVENING

Innovating Materials for the Next Generation: Bringing Practical Applications into the Chemistry Classroom

Sponsored by CHED, Cosponsored by PMSE, POLY and RUBB

SCHB

Division of Small Chemical Businesses

J. Sabol, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Advances in Organic Synthesis: Successes from Academia-Industry Partnerships (see *ORGN*, Tue)

Ask Dr. Safety: Chemical & Occupational Safety in the Cannabis Industry (see *CHAS*, Sun)

Cannabis Law: Navigating Complex Regulatory & Legal Issues in States with Legal Cannabis Programs (see *CHAL*, Wed)

Careers in Chemical Information (see *CINF*, Sun)

Green Chemistry: Theory & Practice (see *CHED*, Sun)

Kathryn C. Hach Award for Entrepreneurial Success: Symposium in honor of David R. Walt (see *ANYL*, Tue)

SOCIAL EVENTS:

SCHB Member's Welcome Social Hour, 5:30 PM: Sat

Coffee & Networking, 8:00 AM: Tue

Luncheon, 11:30 AM: Tue

Reception, 5:00 PM: Tue

BUSINESS MEETINGS:

Business Meeting, 6:30 PM: Sat

Executive Committee Meeting, 7:00 PM: Sat

SUNDAY AFTERNOON

Chemical Angel Network: Chemists Investing in Chemical Companies

Sponsored by BMGT, Cosponsored by PROF‡ and SCHB‡

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

SUNDAY EVENING

Section A

Moscone Center
Halls B/C

Entrepreneurs' Poster Session

G. W. Ruger, *Organizer*

6:00 - 8:00

SCHB **1.** SCHB is the home for entrepreneurs inside the ACS. **A. Rahman**, P.C. Lauro, M. Chorghade, A. Kantak, D.J. Deutsch, J.E. Sabol, J.L. Maclachlan, E.L. Oltermann, R. Chorghade, C.A. Burton, T. Siepmann, P.C. Kearney, G.W. Ruger

SCHB **2.** Chemical Angel Network: Chemists investing in chemical companies. **S.S. White**, M. Vreeke, J.C. Giordan

SCHB **3.** Small chemical businesses providing materials and resources to promote the sciences through outreach activities. **G.W. Ruger**

Entrepreneurial Opportunities in Chemistry

Sponsored by YCC, Cosponsored by BMGT, PROF and SCHB

MONDAY MORNING

Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing

Sponsored by CHAS, Cosponsored by CCS and SCHB‡

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY AFTERNOON

Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing

Sponsored by CHAS, Cosponsored by CCS and SCHB‡

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY EVENING

Section A

Moscone Center
Hall D

Sci-Mix

G. W. Ruger, *Organizer*

8:00 - 10:00

1-3. See previous listings.

‡ *Cooperative Cosponsorship*

TUESDAY MORNING

Section A

Hotel Nikko San Francisco
Nikko Ballroom I

Chemists & Writing for Fun & Profit: Write Your Own Career

Cosponsored by CPRC and PROF

L. M. Balbes, *Organizer, Presiding*

8:00 Networking.

8:30 Introductory Remarks.

8:35 SCHB **4.** How I got my job at C&EN. **L. Wang**

9:05 SCHB **5.** Translating my way around the periodic table. **K.M. Tkaczyk**

9:35 SCHB **6.** How to write your first book without knowing how. **J.E. Brown**

10:05 Intermission.

10:20 SCHB **7.** Taking a leap of faith from one non-traditional career to another. **S.P. Hasford**

10:50 SCHB **8.** Leveraging social media for effective content marketing for corporate and non-profit entities in the chemical enterprise. **J.L. Maclachlan**

11:20 SCHB **9.** Confessions of The Speaking Scientist®: Growing a business that helps scientists communicate when the stakes are high. **N. Milanovich**

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡

TUESDAY AFTERNOON

Section A

Hotel Nikko San Francisco
Nikko Ballroom I

Entrepreneurship in Biotechnology, Advanced Materials, Drug Discovery & Information Systems

Cosponsored by MEDI and PROF

B. A. Bunin, *Organizer*

P. C. Kearney, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 SCHB **10.** Surface-functionalized hollow silica nanoparticles for advanced material applications. **V.O. Rodionov**, H. Ahmad

1:35 SCHB **11.** Xtractite: An inorganic ion-exchange material for sorption of radionuclides and heavy metals. **A.W. Apblett**, E. Kadossov, N.F. Materer, C.K. Perkins

2:05 SCHB **12.** Funding a deep-tech startup: Taking an idea from the back of a napkin to market. **R. Nordsell**, J.H. Melman

2:35 SCHB **13.** Practical wet adhesives and tough resin composites for real business. **K. Ahn**

3:05 Intermission.

3:20 SCHB **14.** 3D tissue-engineered bone marrow, a novel 3D-cell culture model: From basic biological mechanism to a fast revenue generating start-up company with diversified business models. **K. Azab**

3:50 SCHB **15.** Welcome to the real world. **S. Jin**

4:20 SCHB **16.** CDD vault: Building the dominant hosted platform for global hosted commercial and humanitarian drug discovery collaborations. **B.A. Bunin**

4:50 Concluding Remarks.

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡

WEDNESDAY MORNING

Section A

Hotel Nikko San Francisco
Golden Gate

Cannabis: A Growing Sector for Business & Employment

Cosponsored by CHAS

E. M. Pryor, *Organizer*

E. L. Oltermann, *Organizer, Presiding*

8:00 Introductory Remarks.

8:05 SCHB **17.** Emerging opportunity of becoming a cannabis inspector for private and public institutions. **J. Marcu**, E.M. Pryor, M.J. Wilcox, E.L. Oltermann

8:35 SCHB **18.** Employment opportunities in cannabis science: A view into future needs in the cannabis economy and the drivers behind them. **G. Murray**, G.M. Sanz

9:05 SCHB **19.** Chemistry and cannabis: Highlighting the demand for chemists in key roles for a burgeoning industry. **A. Pham**

9:35 Intermission.

9:50 SCHB **20.** Optimizing yield and composition of cannabis extracts of large scale SFE. **M. Roggen**

10:20 SCHB **21.** Scientific and economic challenges facing cannabis testing laboratories. **J.T. Fischedick**, E.M. Pryor

10:50 SCHB **22.** Serving as an educator in the cannabis staffing market. **K. Humiston**, K. Arfsten

11:20 Panel Discussion.

11:50 Concluding Remarks.

CCS

Committee on Chemical Safety

E. Howson, *Program Chair*

SUNDAY AFTERNOON

Best Practices in Selecting & Presenting Safety Training Content

Sponsored by CHAS, Cosponsored by CCS and PRES

Ask Dr. Safety: Chemical & Occupational Safety in the Cannabis Industry

Sponsored by CHAS, Cosponsored by CCS

MONDAY MORNING

Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing

Sponsored by CHAS, Cosponsored by CCS and SCHB‡

MONDAY AFTERNOON

Cannabis: Emerging Challenges in Regulations, Product Analysis & Processing

Sponsored by CHAS, Cosponsored by CCS and SCHB‡

TUESDAY MORNING

Information Flow in Environmental Health & Safety

Sponsored by CHAS, Cosponsored by CCS and CINF‡

TUESDAY AFTERNOON

Information Flow in Environmental Health & Safety

Sponsored by CHAS, Cosponsored by CCS and CINF‡

WEDNESDAY MORNING

What Have We Learned & Where Are We Going: Post-Settlement in the University of California

Sponsored by CHAS, Cosponsored by CCS and PRES

WEDNESDAY AFTERNOON

What Have We Learned & Where Are We Going: Post-Settlement in the University of California

Sponsored by CHAS, Cosponsored by CCS and PRES

CCPA

Committee on Chemistry and Public Affairs

S. Butts, *Program Chair*

SUNDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY MORNING

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

CWD

COMMITTEE ON CHEMISTS WITH DISABILITIES

J. Johnston, *Program Chair*

SUNDAY MORNING

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

SUNDAY AFTERNOON

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, MPPG, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

MONDAY MORNING

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

MONDAY AFTERNOON

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

WEDNESDAY MORNING

Communicating Science in the Twenty-First Century to Diversified Audiences

Sponsored by CHED, Cosponsored by CPRC, CWD and PRES

WEDNESDAY AFTERNOON

Communicating Science in the Twenty-First Century to Diversified Audiences

Sponsored by CHED, Cosponsored by CPRC, CWD and PRES

CCA

COMMITTEE ON COMMUNITY ACTIVITIES

M. McGinnis, *Program Chair*

MONDAY MORNING

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

MONDAY AFTERNOON

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

DAC

Committee on Divisional Activities

R. Bennett, *Program Chair*

SUNDAY MORNING

Young Investigator's Symposium

Sponsored by PMSE, Cosponsored by DAC‡

SUNDAY AFTERNOON

Young Investigator's Symposium

Sponsored by PMSE, Cosponsored by DAC‡

MONDAY MORNING

Young Investigator's Symposium

Sponsored by PMSE, Cosponsored by DAC‡

MONDAY AFTERNOON

Young Investigator's Symposium

Sponsored by PMSE, Cosponsored by DAC‡

CEI

Committee on Environmental Improvement

C. Middlecamp, *Program Chair*

SUNDAY MORNING

Citizens First!

Sponsored by CHED, Cosponsored by CEI

Green Chemistry: Theory & Practice

Sponsored by CHED, Cosponsored by CEI

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

SUNDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Citizens First!

Sponsored by CHED, Cosponsored by CEI

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Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

Integrated & Sustainable Environmental Remediation

Sponsored by ENVR, Cosponsored by CEI

MONDAY MORNING

ACS-CEI Award for Incorporating Sustainability into Chemistry Education

Sponsored by CHED, Cosponsored by CEI

Science for a Sustainable Energy Future

Energy Storage

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENFL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

MONDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Science for a Sustainable Energy Future

Chemical & Biological Conversions Approaches to Energy Conversion

Sponsored by PRES, Cosponsored by BIOL, BIOT, BMGT, CARB, CATL, CEI, CELL, COLL, ENVR, GEOC, I&EC, MEDI, MPPG‡, ORGN and PROF

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Undergraduate Research Posters

Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by CEI and SOCED

TUESDAY MORNING

GSSPC: Water Sustainability

Chemists in Pursuit of Clean Water

Sponsored by CHED, Cosponsored by CEI and PRES

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡

Perspectives on Climate Change Literacy & Education: Local to International

Sponsored by CHED, Cosponsored by CEI and IAC

Innovative Materials & Technologies for Sustainable Water Purification

Adsorption Technologies

Sponsored by ENVR, Cosponsored by CEI

Processes, Technologies & Sensors for Food-Energy-Water Nexus Research

Sponsored by ENVR, Cosponsored by CEI and CHED

TUESDAY AFTERNOON

GSSPC: Water Sustainability

Chemists in Pursuit of Clean Water

Sponsored by CHED, Cosponsored by CEI and PRES

Green Chemistry Adoption: Progressive Changes by Different Industry Sectors

Sponsored by ENVR, Cosponsored by CEI, MEDI, ORGN and SCHB‡

Innovative Materials & Technologies for Sustainable Water Purification

Adsorption Technologies

Sponsored by ENVR, Cosponsored by CEI

Science & Perception of Climate Change

Sponsored by ENVR, Cosponsored by CEI and CHED

WEDNESDAY MORNING

Innovative Materials & Technologies for Sustainable Water Purification

Membrane & Other Treatment

Sponsored by ENVR, Cosponsored by CEI

WEDNESDAY AFTERNOON

Advances in Resource Recovery & Conservation in Water Systems

Sponsored by ENVR, Cosponsored by AGFD, CEI and GEOC

Innovative Materials & Technologies for Sustainable Water Purification

Photocatalytic

Sponsored by ENVR, Cosponsored by CEI

WEDNESDAY EVENING

Contaminants of Emerging Concern in Natural & Engineered Systems

Sponsored by ENVR, Cosponsored by AGRO, ANYL and CEI

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CEI

Innovative Materials & Technologies for Sustainable Water Purification

Sponsored by ENVR, Cosponsored by CEI

Integrated & Sustainable Environmental Remediation

Sponsored by ENVR, Cosponsored by CEI

Science & Perception of Climate Change

Sponsored by ENVR, Cosponsored by CEI and CHED

THURSDAY MORNING

Advances in Resource Recovery & Conservation in Water Systems

Sponsored by ENVR, Cosponsored by AGFD, CEI and GEOC

Innovative Materials & Technologies for Sustainable Water Purification

Catalytic

Sponsored by ENVR, Cosponsored by CEI

THURSDAY AFTERNOON

Advances in Resource Recovery & Conservation in Water Systems

Sponsored by ENVR, Cosponsored by AGFD, CEI and GEOC

Innovative Materials & Technologies for Sustainable Water Purification

Catalytic & Electrochemical

Sponsored by ENVR, Cosponsored by CEI

‡ *Cooperative Cosponsorship*

ETHX

Committee on Ethics

K. Vitense, *Program Chair*

MONDAY AFTERNOON

The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit

Sponsored by CINF, Cosponsored by CHED, CPRM and ETHX‡

IAC

International Activities Committee

E. Tratras Contis, *Program Chair*

SOCIAL EVENTS:

Networking Globally: Helping Chemistry Students Find Success in Careers and Study Abroad, 4:30 PM: Sun

International Welcome Reception, 5:30 PM: Sun

SUNDAY MORNING

Section A

Hotel Nikko San Francisco

Carmel II

Blending Chemistry & Culture: Undergraduate Research Abroad through ACS IREU Program

Cosponsored by CHED

L. Brown, *Organizer*

C. LaPrade, *Organizer, Presiding*

9:15 Introductory Remarks.

9:25 IAC **1.** My summer experience: Researching water oxidation catalysts and experiencing the beauty of Italy. **R. Hutchinson**

9:45 IAC **2.** La ragazza in Italia: The p-docelyloxybenzyldimethylammine oxide (pDoAO) gel as pH sensitive artificial gland. **N.E. Caldero-Rodriguez**

10:05 IAC **3.** Multiple reaction conditions & multiple reasons why I need to travel more. **S. Fusi**

10:25 IAC **4.** Optics in Umbria: Investigating nanoparticles and fluorescence in the land of pizza and piazzas. **R. Warnock**, G. Massaro, L. Latterini

10:45 Intermission.

11:00 IAC **5.** Fascinating summer with research in organic solar cells, exploring Glasgow and the beautiful highlands of Scotland. **M. Matar Abed**

11:20 IAC **6.** Bagpipes, highlands, and cholesterol functionalized gold nanoparticles. **R. Kress**

11:40 IAC **7.** Performing synthesis and gaining cultural awareness in Germany. **E. Janeira**

12:00 IAC **8.** Summer in Germany: Exploring Europe, making friends, and synthesizing peptides. **M. Gaviria**

Chemistry of Korean Foods & Beverages

Sponsored by AGFD, Cosponsored by IAC

SUNDAY AFTERNOON

Section A

Hotel Nikko San Francisco

Carmel II

Blending Chemistry & Culture: Undergraduate Research Abroad through ACS IREU Program

Cosponsored by CHED

L. Brown, *Organizer*

C. LaPrade, *Organizer, Presiding*

1:30 IAC **9.** Prost to polymers and proteins: A summer spent exploring the world from the nano to global scale. **M.J. Austin**, S. Schubert, M. Leiske, A. Traeger, U.S. Schubert

1:50 IAC **10.** Summer in Germany: Improving lithium ion battery technology and exploring Europe. **N. James**

2:10 IAC **11.** Summer in Germany: Computational electrochemistry, magnesium batteries, and self-discovery. **A.T. Berry**

2:30 IAC **12.** Applying global solutions to bacterial infections: Synthesis of cystobactamide 861-2. **A. Deyett**

2:50 IAC **13.** International research experience: Investigating the biosynthesis of terrein in *Aspergillus terreus* and experiencing Germany. **M. Villanueva**

3:10 IAC **14.** Undergraduate research in Singapore: Explorations of protein-protein interactions and Southeast Asia. **K. Senn**, B. Woo, S. Chng

3:30 IAC **15.** Exploring southeast Asia and biogenic synthesis of silver nanoparticles. **L. Browder**, D. Yong Wei Ying, W.S. Chin

3:50 IAC **16.** MOFs to mee soto: A summer at the National University of Singapore. **M. Molenda**

4:10 Concluding Remarks.

Chemistry of Korean Foods & Beverages

Sponsored by AGFD, Cosponsored by IAC

MONDAY MORNING

Section A

Hotel Nikko San Francisco

Carmel I

Teaching, Researching & Community Building in the Global Chemical Enterprise

Cosponsored by BMGT, ENVR, I&EC, PRES and PROF

L. Brown, P. Kostiuk, E. Tratras Contis, *Organizers*, *Presiding*

9:00 Introductory Remarks.

9:15 IAC **17.** Festival De Química: A successful model to communicate the value and impact of chemistry to local communities. **I. Montes-González**, L. Brown

9:45 IAC **18.** Beyond the lab: An international Younger Chemists Network in the works. **J. Breffke**, P. Kostiuk

10:15 IAC **19.** Fighting chemofobia through community building: Lessons learned from the local, national, and international arenas. **C. Janaky**, L. Brown

10:45 Intermission.

11:00 IAC **20.** Global perspectives of Citizen Science. **I.T. Urasa**, L. Brown

11:30 IAC **21.** The challenges and benefits of international research collaborations for undergraduate institutions. **T.W. Hanks**, P. Kostiuk

12:00 Intermission.

12:30 Panel Discussion.

MONDAY AFTERNOON

Section A

Hotel Nikko San Francisco

Carmel I

Teaching, Researching & Community Building in the Global Chemical Enterprise

Cosponsored by BMGT, ENVR, I&EC, PRES and PROF

L. Brown, P. Kostiuk, E. Tratras Contis, *Organizers*, *Presiding*

1:30 IAC **22.** Green chemistry education in Brazil: The 2016 Global Innovation Imperatives (GIi) program from the perspective of a chemist in industry. **S.C. Nanita**, P. Kostiuk

2:00 IAC **23.** Sharing best practices in the global chemical enterprise. **E. Tratras Contis**, L. Brown

2:30 Intermission.

2:45 IAC **24.** Developing an ACS international chapter in the presence of a strong local chemical society. **S. McAlpine**, P. Kostiuk

3:15 IAC **25.** Malta Conference Series: Measuring the success of science diplomacy. **Z.M. Lerman**, **M.Z. Hoffman**

3:45 Concluding Remarks.

International & Multicultural Perspective

Sponsored by CHED, Cosponsored by IAC

TUESDAY MORNING

Perspectives on Climate Change Literacy & Education: Local to International

Sponsored by CHED, Cosponsored by CEI and IAC

WEDNESDAY MORNING

Research on Learning in the Lab

Sponsored by CHED, Cosponsored by IAC‡

Research on Learning in the Lab

Sponsored by CHED, Cosponsored by IAC‡

LSAC

Committee on Local Section Activities

M. Rudd, *Program Chair*

SUNDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

MONDAY MORNING

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

MONDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

CMA

Committee on Minority Affairs

J. Sarquis, *Program Chair*

SUNDAY MORNING

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

SUNDAY AFTERNOON

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Sponsored by WCC, Cosponsored by CHED, CMA and PROF

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodologies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

MONDAY MORNING

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

MONDAY AFTERNOON

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

TUESDAY MORNING

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Sponsored by WCC, Cosponsored by CHED, CMA and PROF

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Saundra Y. McGuire

Sponsored by CHED, Cosponsored by CMA and WCC

TUESDAY AFTERNOON

Advancing Undergraduate Research

Focus on Early Access to Research & Broadening Participation of Under-Represented Groups

Sponsored by CHED, Cosponsored by CMA‡, PROF‡ and WCC

WEDNESDAY MORNING

Advancing Undergraduate Research

Sponsored by CHED, Cosponsored by CMA, PROF and WCC

CPRM

Committee on Patents and Related Matters

S. Shah, *Program Chair*

MONDAY AFTERNOON

The Write Thing to Do: Ethical Considerations in Authorship & the Assignment of Credit

Sponsored by CINF, Cosponsored by CHED, CPRM and ETHX‡

CPRC

Committee on Public Relations and Communications

D. Nelson, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Chemists & Writing for Fun & Profit: Write Your Own Career (see *SCHB, Tue*)

Communicating Science in the Twenty-First Century to Diversified Audiences (see *CHED, Wed*)

Science & Perception of Climate Change (see *ENVR, Tue, Wed*)

Perspectives on Climate Change Literacy & Education; Local to International (see *CHED, Tue*)

Citizens First! (see *CHED, Sun*)

Chemistry through the Eyes of Non-Chemists (see *HIST, Mon, Tue*)

EVENTS:

Workshop—Getting Involved: Chemistry Ambassadors' Forum, 2:00 PM: Sun

SUNDAY AFTERNOON

Section A

Moscone Center

135

Hollyweird Chemistry

Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

D. J. Nelson, *Organizer, Presiding*

K. Grazier, D. A. Kirby, *Presiding*

1:10 Introductory Remarks.

1:15 CPRC **1.** Science in the TV show Breaking Bad. **D.J. Nelson**

1:45 CPRC **2.** Bridging the worlds of science fiction and science fact on Star Trek. **A. Bormanis**

2:15 CPRC **3.** How *"The Universe"* is made. **C. Campbell**

2:45 CPRC **4.** NOVA's *"Hunting the Elements"* and other chemistry projects. **C. Schmidt**, P. Rosenstein

3:15 CPRC **5.** Science and science fiction: The boundary between fantasy and futurism. **J. Colwell**

3:45 CPRC **6.** Science as a human story. **S.E. Lyons**

4:15 Panel Discussion.

MONDAY MORNING

Section A

Moscone Center

135

Hollyweird Chemistry

Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

D. J. Nelson, *Organizer, Presiding*

M. A. Griep, *Presiding*

9:00 CPRC **7.** Hollyweird scientists. **K. Grazier**

9:30 CPRC **8.** Correctness, creativity, and compromise: The art of putting good science into great television. **J.G. Sotos**

10:00 CPRC **9.** Role of scientific integrity in cinematic and televised science. **D.A. Kirby**

10:30 CPRC **10.** Who is speaking? Film and TV as part of an on-going dialogue between science and society. **E. Stengler**

11:00 CPRC **11.** Too many geeks? **S. Cass**

11:30 Panel Discussion.

Space Chemistry: How it Helps Space Exploration

Sponsored by YCC, Cosponsored by CPRC and PROF

MONDAY AFTERNOON

Section A

Moscone Center

135

Hollyweird Chemistry

Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

D. J. Nelson, *Organizer, Presiding*

J. G. Sotos, *Presiding*

1:15 CPRC **12.** Teaching chemistry using popular media. **J.G. Goll**

1:45 CPRC **13.** How to teach chemistry using Movie Wow! **M.A. Griep**, M. Mikasen

2:15 CPRC **14.** Effective science communication in the popular media. **J.J. Grbic**

2:45 CPRC **15.** Making science humerus (pun intended). **N. Reagan**

3:15 CPRC **16.** This is your brain on Hollywood. Any questions? **J. Cail**

3:45 Panel Discussion.

Space Chemistry: How it Helps Space Exploration

Sponsored by YCC, Cosponsored by CPRC and PROF

TUESDAY MORNING

Chemists & Writing for Fun & Profit: Write Your Own Career

Sponsored by SCHB, Cosponsored by CPRC and PROF

WEDNESDAY MORNING

Communicating Science in the Twenty-First Century to Diversified Audiences

Sponsored by CHED, Cosponsored by CPRC, CWD and PRES

WEDNESDAY AFTERNOON

Communicating Science in the Twenty-First Century to Diversified Audiences

Sponsored by CHED, Cosponsored by CPRC, CWD and PRES

COMSCI

Committee on Science

M. Kociolek, *Program Chair*

MONDAY AFTERNOON

Section A

Moscone Center

132

Chemical Innovation Partnerships: Industry-University Success Stories

Cosponsored by BMGT

M. G. Kociolek, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 COMSCI **1.** Successful models and key principles in university-industry partnerships. **A. Boccanfuso**

1:35 COMSCI **2.** Open Laboratory initiatives and their role in innovation partnerships. **M.G. Kociolek**

2:05 Intermission.

2:15 COMSCI **3.** Successful university partnerships in the pharmaceutical industry. **C.J. Welch**

2:45 COMSCI **4.** Government's role in public-private partnerships. **G. Wang**

3:15 Panel Discussion.

SCC

Senior Chemists Committee

T. Beattie, *Program Chair*

SUNDAY AFTERNOON

Golden Age of Industrial Chemistry

Sponsored by HIST, Cosponsored by SCC and YCC

‡ *Cooperative Cosponsorship*

SOCED

Society Committee on Education

M. Roslonowski, *Program Chair*

SOCIAL EVENTS:

Networking Social with Graduate School Recruiters, 1:00 PM: Sun

Undergraduate Social, 8:30 PM: Sun

Undergraduate Speed Networking with Chemistry Professionals, 4:00 PM: Mon

EVENTS:

SciBabe: Chemistry Blogger, 4:00 PM: Sun

Student Awards Ceremony, 7:00 PM: Sun

Chemistry & the Environment Film Series, 12:00 PM: Mon

SUNDAY MORNING

Section A

San Francisco Marriott Marquis
Golden Gate A

Frontiers in Nanoscience

Cosponsored by POLY

M. C. Roslonowski, *Organizer, Presiding*

9:30 Introductory Remarks.

9:45 SOCED **1.** Donor-Acceptor molecules for organic photovoltaics. **M.C. Stefan**

10:10 SOCED **2.** Incorporating Diels-Alder chemistry to prepare thermally-responsive materials. M. Markmann, M.R. Martinez, T. Kleine, M. Meyersohn, C. Gregory, T. Colt, **P.J. Costanzo**

10:30 SOCED **3.** Single molecule/aggregate spectroscopy for plastic semiconducting polymers. **Z. Hu**

10:50 SOCED **4.** Withdrawn.

11:10 SOCED **5.** Degradable conjugated polymers: New biomaterials for biological labeling, sensing, and delivery. **J. Moon**

11:30 SOCED **6.** Directed self-assembly: A new frontier for nanolithography. **A. Baruth**

11:50 Q&A.

12:05 Concluding Remarks.

Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

SUNDAY AFTERNOON

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

MONDAY MORNING

Section A

San Francisco Marriott Marquis
Golden Gate A

Chemistry of Fermented Beverages

M. C. Roslonowski, *Organizer, Presiding*

10:00 Introductory Remarks.

10:10 SOCED **7.** Chemistry in homebrewing. **R. Burns**

10:45 Q&A.

10:55 SOCED **8.** How offering a beer course can make you famous and infamous. **M.C. Roslonowski**

11:30 Q&A.

11:40 SOCED **9.** Beer, chemistry and the secrets of the universe. **M.B. Cichowicz**

12:15 Q&A.

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

MONDAY AFTERNOON

Section A

San Francisco Marriott Marquis
Golden Gate A

Eminent Scientist Lecture with Dr. Carolyn Bertozzi

Cosponsored by MEDI

M. C. Roslonowski, *Organizer, Presiding*

2:30 Introductory Remarks.

2:40 SOCED **10.** What life and research share in common: Finding opportunity in failure. **C.R. Bertozzi**

3:40 Concluding Remarks.

3:55 Q&A.

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

Undergraduate Research Papers

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Agricultural & Food Chemistry

Sponsored by CHED, Cosponsored by AGFD‡ and SOCED‡

Undergraduate Research Posters

Agricultural & Food Chemistry

Sponsored by CHED, Cosponsored by AGFD‡ and SOCED‡

Undergraduate Research Posters

Analytical Chemistry

Sponsored by CHED, Cosponsored by ANYL and SOCED

Undergraduate Research Posters

Biochemistry

Sponsored by CHED, Cosponsored by BIOL and SOCED

Undergraduate Research Posters

Biotechnology

Sponsored by CHED, Cosponsored by BIOT and SOCED

Undergraduate Research Posters

Chemical Education

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Computational Chemistry

Sponsored by CHED, Cosponsored by COMP and SOCED

Undergraduate Research Posters

Environmental Chemistry

Sponsored by CHED, Cosponsored by ENVR and SOCED

Undergraduate Research Posters

Geochemistry

Sponsored by CHED, Cosponsored by GEOC and SOCED

Undergraduate Research Posters

Green Chemistry & Sustainability

Sponsored by CHED, Cosponsored by CEI and SOCED

Undergraduate Research Posters

Inorganic Chemistry

Sponsored by CHED, Cosponsored by INOR and SOCED

Undergraduate Research Posters

Medicinal Chemistry

Sponsored by CHED, Cosponsored by MEDI and SOCED

Undergraduate Research Posters

Nanochemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Organic Chemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Physical Chemistry

Sponsored by CHED, Cosponsored by SOCED

Undergraduate Research Posters

Polymer Chemistry

Sponsored by CHED, Cosponsored by PMSE, POLY and SOCED

MONDAY EVENING

Successful Student Chapters

Sponsored by CHED, Cosponsored by SOCED

TUESDAY MORNING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY AFTERNOON

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY EVENING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WCC

Women Chemists Committee

K. Woznack and R. Cole, *Program Chairs*

SOCIAL EVENTS:

Breakfast, 7:30 AM: Mon

Just Cocktails, 4:00 PM: Mon

Luncheon, 12:00 PM: Tue

EVENTS:

Poster Session, 11:00 AM: Tue

SUNDAY MORNING

High School Program

Sponsored by CHED, Cosponsored by WCC

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Emerging Applications in Inorganic Chemistry: Energy, Materials, Catalysis & Spectroscopy

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Polymer Synthesis

Sponsored by PMSE, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Single Crystal Catalysis

Sponsored by CATL, Cosponsored by COLL and WCC

Lanthanide & Actinide Chemistry

Sponsored by INOR, Cosponsored by WCC

SUNDAY AFTERNOON

Section A

Hotel Nikko San Francisco

Monterey II

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Cosponsored by CHED, CMA and PROF

K. A. Woznack, *Organizer*

E. A. Nalley, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 WCC **1.** Encouraging true grit women in science: The story of a grit grinder. **R.A. Woodall**

2:00 WCC **2.** Paying it forward in mentoring. **A.F. Charlebois**

2:25 WCC **3.** POM (Power of Mentorship): The role mentorship in chemical sciences played in my life. **F.F. Minter**

2:50 Intermission.

3:00 WCC **4.** Encouragement. **R. Libby**

3:25 WCC **5.** What Women Can Do^{tm}: Encouraging and retaining women in STEM. **J.L. Bryant**

3:50 WCC **6.** Reaching gender equity for women of color in STEM. The importance of role models and mentors. **T. Thomas**, J.M. Iriarte-Gross

4:15 WCC **7.** Mentors, role models, and advisors: Distinctions, examples, and ethical issues. **S.C. Greer**

4:40 Concluding Remarks.

High School Program

Sponsored by CHED, Cosponsored by WCC

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Novel Reactions, Methodolgies & Syntheses in Organic Chemistry

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Advances in Organic Solar Cells

Sponsored by PMSE, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Single Crystal Catalysis

Sponsored by CATL, Cosponsored by COLL and WCC

SUNDAY EVENING

F. Albert Cotton Award in Synthetic Inorganic Chemistry: Symposium in honor of Pingyun Feng

Sponsored by INOR, Cosponsored by WCC

MONDAY MORNING

Section A

Hotel Nikko San Francisco

Monterey II

Celebrating 90 years of the WCC: Reflections of Past Chairs

Cosponsored by PRES and PROF‡

R. S. Cole, *Organizer*

T. N. Horton, *Organizer, Presiding*

L. S. Sremaniak, *Presiding*

9:15 Introductory Remarks.

9:25 WCC **8.** Looking at life from both sides now. **F.K. Wood-Black**

9:45 WCC **9.** WCC: Reaching out. **C. Ribes**

10:05 WCC **10.** Partnerships, awards and taboo topics, oh my! Happy Birthday WCC! **A.F. Charlebois**

10:25 Intermission.

10:40 WCC **11.** Back to the 80s... or not? **M.A. Cavanaugh**

11:00 WCC **12.** Transformation of the Women's Chemists Committee: 1995-1997. **C. Bodurow**

11:20 WCC **13.** Sustainable programs to encourage and retain women chemists: Efforts from the Women Chemists Committee (WCC). **J.L. Bryant**

11:40 WCC **14.** Rising stars in the WCC Hall of Fame: Perspectives on recognizing mid-career chemists. **J. Cohen**

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Symposium in honor of Marcy H. Towns

Sponsored by CHED, Cosponsored by WCC

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Frontiers in Analytical & Physical Chemistry: From Atmospheric to Atomic Discoveries

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Novel Organic Materials

Sponsored by PMSE, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Nanocatalysis

Sponsored by CATL, Cosponsored by COLL and WCC

MONDAY AFTERNOON

Section A

Hotel Nikko San Francisco

Monterey II

Rising Star Award Symposium

Cosponsored by BIOL and PRES

M. A. Kane, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 WCC **15.** Novel liquid-like nano-scale hybrid materials with tunable chemical and structural properties for combined CO2 capture and conversion. **A.A. Park**

1:55 WCC **16.** Catalyzing innovation – the diverse elements of my career. **B.A. Kilos**

2:15 WCC **17.** Inspiration from nature: Mentors and molecules. **E.E. Carlson**

2:35 Intermission.

2:40 WCC **18.** From a farm kid to a scientist and the analyses along the way. **E.S. Baker**, X. Zheng, N. Aly, X. Zhang, K. Burnum-Johnson, D. Orton, Y. Ibrahim, R. Smith

3:00 WCC **19.** Stay on target: Isozyme-specific first responders in precision electrophile signaling. **Y. Aye**

3:20 WCC **20.** Biological chemistry of f-elements: From decontamination to targeted radiotherapy. **R.J. Abergel**

3:40 Concluding Remarks.

ACS Award for Achievement in Research for the Teaching & Learning of Chemistry: Symposium in honor of Marcy H. Towns

Sponsored by CHED, Cosponsored by WCC

LGBT Graduate & Postdoctoral Student Chemistry Research Symposium

Advances in Medicinal & Biological Chemistry: From Therapeutics to Education

Sponsored by PROF, Cosponsored by ANYL‡, BIOL‡, CHED, CMA, COLL, COMP, CWD, ENVR, INOR‡, MEDI, MPPG, ORGN, PHYS, PMSE‡, POLY, PRES‡ and WCC

ACS Award in Applied Polymer Science: Symposium in honor Zhenan Bao

Frontiers in Organic & Flexible Electronics

Sponsored by PMSE, Cosponsored by WCC

ACS Award in Surface Chemistry: Symposium in honor of Cynthia M. Friend

Honoring the Contribution to Nanocatalysis

Sponsored by CATL, Cosponsored by COLL and WCC

TUESDAY MORNING

Section A

Hotel Nikko San Francisco

Monterey II

The Importance of Role Models & Mentors in Reaching Gender Equity in Chemical Sciences: A Symposium in Honor of Judith Iriarte-Gross

Cosponsored by CHED, CMA and PROF

E. A. Nalley, K. A. Woznack, *Organizers*

R. A. Woodall, *Presiding*

8:30 Introductory Remarks.

8:35 WCC **21.** Why STEM is still a four-letter word for women. **E.A. Nalley**

9:00 WCC **22.** Mentors and role models: Stories from the field. **K.M. Schulz**

9:25 WCC **23.** Expanding Your Horizons (EYH) addresses equity issues for girls in STEM. **P.R. Pulley**

9:50 Intermission.

10:00 WCC **24.** Challenges and opportunities for leadership in the 21st century. **D.G. Schmidt**

10:25 WCC **25.** Underrepresentation of women in science and what we can do about it. **D.J. Nelson**

10:50 WCC **26.** Reaching gender equity in the chemical sciences: The importance of role models and mentors. Fortune cookie wisdom for women in the chemical sciences. **J.M. Iriarte-Gross**

ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences: Symposium in honor of Saundra Y. McGuire

Sponsored by CHED, Cosponsored by CMA and WCC

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

TUESDAY AFTERNOON

ACS Chemical Biology Award Symposium

Sponsored by BIOL, Cosponsored by WCC

ACS Award Lectures

Sponsored by COLL, Cosponsored by CATL and WCC

ACS Award for Computers in Chemical & Pharmaceutical Research: Symposium in honor of Yvonne C. Martin

Sponsored by COMP, Cosponsored by BIOL, MEDI and WCC

Frank H. Field & Joe L. Franklin Award for Outstanding Achievement: Symposium in Honor of Vicki H. Wysocki

Sponsored by ANYL, Cosponsored by WCC

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

Advancing Undergraduate Research

Focus on Early Access to Research & Broadening Participation of Under-Represented Groups

Sponsored by CHED, Cosponsored by CMA‡, PROF‡ and WCC

Advancing Undergraduate Research

Focus on Early Access to Research & Broadening Participation of Under-Represented Groups

Sponsored by CHED, Cosponsored by CMA‡, PROF‡ and WCC

‡ *Cooperative Cosponsorship*

WEDNESDAY MORNING

Nobel Laureate Signature Award for Graduate Education in Chemistry: Symposium in honor of Junqi Li & Martin D. Burke

Sponsored by ORGN, Cosponsored by WCC

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

Lanthanide & Actinide Chemistry

Sponsored by INOR, Cosponsored by WCC

Advancing Undergraduate Research

Sponsored by CHED, Cosponsored by CMA, PROF and WCC

WEDNESDAY AFTERNOON

Chemical Probes for Bacterial Imaging

Sponsored by BIOL, Cosponsored by WCC

Biomass & Biofuel Processing

Sponsored by ENFL, Cosponsored by CELL, MPPG‡ and WCC

THURSDAY MORNING

Lanthanide & Actinide Chemistry

Sponsored by INOR, Cosponsored by WCC

THURSDAY AFTERNOON

Lanthanide & Actinide Chemistry

Sponsored by INOR, Cosponsored by WCC

YCC

Younger Chemists Committee

D. Williams, *Program Chair*

SUNDAY AFTERNOON

Section A

Moscone Center

2000

Starting a Successful Research Program at a PUI

Cosponsored by PROF

Financially supported by Council on Undergraduate Research

M. L. Druelinger, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 YCC **1.** What is undergraduate research and why do research at a predominantly undergraduate institution? **M.R. Malachowski**

1:25 YCC **2.** Collaborative research with undergraduates: Research project and research group design. **M.R. Malachowski**

1:45 YCC **3.** Balancing teaching, research, service and life in the context of Primarily Undergraduate Institutions (PUIs). **B.L. Gourley**

2:05 YCC **4.** Art and necessity of gaining internal support from institutional administrators. **M.L. Druelinger**

2:25 Intermission.

2:40 YCC **5.** Undergraduate new investigator grants at the ACS Petroleum Research Fund. **T. Clancy**

3:05 YCC **6.** Funding opportunities at the National Science Foundation of particular interest to faculty at Primarily Undergraduate Institutions (PUIs). **C.A. Bessel**

3:35 YCC **7.** Writing more competitive grant proposals. **C.A. Bessel**

3:55 YCC **8.** Finding small grant opportunities to jump-start your research. **B.L. Gourley**

4:15 Q&A & Panel Discussion.

4:35 Concluding Remarks.

Golden Age of Industrial Chemistry

Sponsored by HIST, Cosponsored by SCC and YCC

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

SUNDAY EVENING

Section A

Moscone Center

2000

Entrepreneurial Opportunities in Chemistry

Cosponsored by BMGT, PROF and SCHB

J. Schmitt, J. Schwarzbach, *Organizers*, *Presiding*

5:00 Introductory Remarks.

5:10 YCC **9.** Cofounding a biochemical startup. **P.V. Robinson**

5:35 YCC **10.** Working with academia and startups. **J.C. Ramos**

6:00 YCC **11.** Cofounding a materials startup. **L. Brockway**

6:25 YCC **12.** Working with national labs and the government for your startup. **X. Wei**

6:50 Panel Discussion.

7:30 Concluding Remarks.

MONDAY MORNING

Section A

Moscone Center

2000

Space Chemistry: How it Helps Space Exploration

Cosponsored by CPRC and PROF

F. Darvas, R. F. Hirsch, A. E. Pavlath, *Organizers*, *Presiding*

8:00 Introductory Remarks.

8:05 YCC **13.** General chemistry of the planets. **L.B. Roberson**

8:35 YCC **14.** Chemistry in space: Demands, perspectives and tools. R.V. Jones, **F. Darvas**

9:05 YCC **15.** Pharmacy on demand by synthesis in the space. **F. Gupton**

9:35 YCC **16.** Polymers and nanostructuring in flow synthesis: Space chemistry perspective. **R.C. Advincula**

10:05 Intermission.

10:20 Introduction of Dr. Shannon Lucid.

10:25 YCC **17.** Following chemistry into space. **S. Lucid**

10:55 YCC **18.** Advanced synthesis in micro-structured flow reactors: From rocket propellants to future space explorations. **S. Loebbecke**

11:25 YCC **19.** Polyimide and polyamide aerogels: Lightweight, multifunctional materials for aerospace applications. **M. Meador**

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

MONDAY AFTERNOON

Section A

Moscone Center

2000

Space Chemistry: How it Helps Space Exploration

Cosponsored by CPRC and PROF

F. Darvas, R. F. Hirsch, A. E. Pavlath, *Organizers*, *Presiding*

1:30 YCC **20.** Flow chemistry: An enabler for space chemistry. **V. Hessel**, T. Noel

2:00 YCC **21.** Utilizing flow chemistry to harness high energy photochemical reactions in space. **A.B. Beeler**

2:30 YCC **22.** Challenges and opportunities regarding the (photo) electrochemical transformation of CO_2 on the Mars. **C. Janaky**

3:00 Intermission.

3:15 YCC **23.** Electrochemistry: Reagentless oxidations and reductions in space. **T. Wirth**

3:45 YCC **24.** Flow fine synthesis: High yielding and selective organic synthesis in space by flow methods. **S. Kobayashi**

4:15 YCC **25.** Martian chemical and mineralogical analysis with ChemCam and SuperCam. **S.M. Clegg**, R. Wiens, S. Maurice, O. Gasnault

Hollyweird Chemistry

Sponsored by CPRC, Cosponsored by AGRO, CARB, CCPA, CEI, CHED, ENFL, HIST, LSAC, NUCL, POLY, SCHB, SOCED and YCC

Fundamentals of Chemistry Outreach Education: From Program Design to Assessment

Sponsored by CHED, Cosponsored by CCA, LSAC, SOCED and YCC

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY MORNING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY AFTERNOON

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

TUESDAY EVENING

Excellence in Graduate Polymer Research

Sponsored by POLY, Cosponsored by PRES, PROF, SOCED and YCC

WEDNESDAY MORNING

Looking Beyond Your Current Boundaries: What's the Next Step?

Academic Route: PhD to Postdoc to Ass. Prof.

Sponsored by PROF, Cosponsored by BMGT and YCC

WEDNESDAY AFTERNOON

Looking Beyond Your Current Boundaries: What's the Next Step?

Industrial Route: PhD, Postdoc, Scientist

Sponsored by PROF, Cosponsored by BMGT and YCC

THURSDAY MORNING

Young Investigators in Nuclear & Radiochemistry

Sponsored by NUCL, Cosponsored by YCC

THURSDAY AFTERNOON

Young Investigators in Nuclear & Radiochemistry

Sponsored by NUCL, Cosponsored by YCC

Technical program information known at press time. The official technical program for the 253rd ACS National Meeting is available at: www.acs.org/SanFran2017

EXPOSITION HIGHLIGHTS

SEE WHAT'S NEW INSIDE THE EXPOSITION. Visit the ACS National Exposition at the Moscone Center, Halls B/C, from Sunday, April 2, through Tuesday, April 4. The show hours will be Sunday, 6:00 to 8:30 PM, and Monday and Tuesday, 9:00 AM to 5:00 PM. Companies will showcase services, instruments, books, computer hardware, scientific software, and an array of chromatographic, lab, and safety equipment. Technical personnel will give demonstrations, answer questions, and discuss your needs and interests.

Visit the revamped ACS Career Fair where you'll meet recruiters from top employers like KAUST, Brewer Science, Gilead and many more. Create an online profile and upload your résumé to our database where recruiters can schedule in-person interviews with you. While at the Career Fair, network with potential employers and drop-off your résumé, attend Career Pathways Workshops, and meet with ACS Career Consultants.

Also, join us at the ACS booth in the middle of the exposition floor, where ACS staff members will present the many benefits, services, products, and merchandise offered by ACS.

Online exposition. The online exposition is a component within the exhibitor directory that enables attendees to view videos, press releases, brochures, and flyers of participating exhibitors. Access the online exposition at www.acs.org/sanfran2017 to learn more about exhibiting companies and download product information that meets your needs.

Free exhibitor workshops. Free workshops will be hosted by exhibitors on the exposition floor and in private rooms inside the Moscone Center. These workshops will introduce new products and services, build skills with specific tools and techniques, and highlight innovative applications that may improve your productivity. Register at www.acs.org/sanfran2017 to reserve your seat.

Presentations & special events. Join us on Sunday from 6:00 to 8:30 PM for the attendee welcome reception. Take an afternoon break on Tuesday from 3:00 to 5:00 PM and visit the exhibitors before the exposition closes. Access the mobile app, play a game with participating exhibitors and win special prizes!

Internet & technology. Get free internet access and leave messages for one another at the meeting mail terminals inside the town center. Enjoy free Wi-Fi service at designated areas in the Moscone Center.

Admission requirements & expo-only registration. Exposition admission is complimentary for all national meeting registrants; however, you are required to wear your badge. Individuals who want to visit the exhibits without registering for the technical component of the national meeting can obtain an expo-only badge for $60. Students with school identification can obtain an expo-only badge for $30. Registration can be handled online or in person at ACS attendee registration at the Moscone Center, North Lobby, and at our satellite registration areas at the Hilton San Francisco Union Square, and Grand Hyatt San Francisco.

ACS Exposition

EXHIBITORS

The following list of exhibitors, as of Feb. 11, is the property of the American Chemical Society. Any unauthorized use of this list, or any part thereof, either directly or indirectly, is strictly prohibited.

Visit the Online ACS National Exposition at www.acs.org/sanfran2017 to download the updated exhibitor list and access product information.

101, 375 South End Avenue, Apt. 9G, New York, NY, United States 10280, 917-587-7883, Internet: www.101edu.co *101 builds subject-specific classroom engagement tools that promote active learning in college STEM courses. Our first product for chemistry courses, Chem101, was piloted with 2000 students across 8 schools in Fall 2016 including Carnegie Mellon, Columbia University, and the University of Cincinnati.* **1530**

abcr GmbH, Im Schlehert 10, Karlsruhe, Germany 76187, +49 721 950 61101, fax: +49 721 950 6133, Internet: www.abcr.de *With abcr, you have access to over 260,000 products from the organic, organometallic and inorganic specialty chemicals area.*
- *R&D services: custom synthesis, research projects*
- *Production: research, syntheses, scale-up, pilot and commercial plant in our production facilities*
- *Semi bulk / bulk business*
- *Catalogue business: procurement and sales of specialty chemicals* **1718**

Accela ChemBio Co. Ltd., 9883 Pacific Heights Blvd., Suite H, San Diego, CA, United States 92121, 858-699-3322, fax: 858-769-6322 or 858-876-1948, e-mail: info@accelachem.com, Internet: www.accelachem.com *Accela ChemBio focus on design, synthesis, manufacture R&D chemicals and pharmaceutical intermediates for worldwide scientific research institutions and industrial development corporations. Since founding in 2007, Accela are providing high-quality, innovative products to over 3,000+ valuable customers in 38 countries. We run ISO9001-Quality-System daily, and certified by Tuv since 2010.* **418**

Ace Glass, Inc., 1430 N. West Blvd., PO Box 688, Vineland, NJ, United States 08360, 800-223-4524, fax: 800-543-6752, e-mail: sales@aceglass.com, Internet: www.aceglass.com *Ace Glass Incorporated has been a leader and innovator of scientific glassware, lab equipment and glass apparatus for over 80 years. Ace Glass provides a wide variety of quality U.S. manufactured standard and custom scientific glassware, including reactors engineered to any customer specifications from 100mL-200L.* **518**

ACS Career Fair Recruiters

ACS Career Consultants	**2028**
Aramco Services Company	**1825**
Brewer Science, Inc.	**1927**
Central Intelligence Agency (CIA)	**1931**
Getson & Schatz, P.C.	**2026**
Gilead	**1735**
Institute for Basic Science (IBS)	**1934**
KAUST	**1725**
Lanzhou University	**1933**
Merck & Co.	**1925**
Open Eye	**2030**
ORAU	**1935**
Sasol	**2034**

ACS Career Navigator, 1155 16th Street, NW, Washington, DC, United States 20036, 202-872-6031, e-mail: k_redmond@acs.org, Internet: https://www.acs.org/content/acs/en/careers/career-navigator.html **725**

ACS Committee on Chemical Health & Safety, P.O. Box 152329, San Diego, CA, United States 92195, 619-990-4908, Internet: www.acs.org/safety *The ACS Committee on Chemical Safety and the Division of Chemical Health and Safety provide this opportunity for you to learn more about chemical safety within the ACS and to have chemical safety experts answer your questions.* **1125**

ACS Division of Small Chemical Businesses (SCHB), 4344 Moorpark Ave., Ste # 1, San Jose, CA, United States 95129, 408-834-8597, fax: 408-351-7900, e-mail: expo-booth@acs-schb.org, Internet: www.acs-schb.org *The ACS Division of Small Chemical Businesses (SCHB) has objectives "To aid in the formation, development, and growth of small chemical businesses." SCHB helps chemists working in small enterprises, including self-employed, with the legal, social, educational, legislative, regulatory, and economic aspects of their unique professional status.* **1329**

ACS Education, 1155 16th Street, NW, Washington, DC, United States 20036, 202-872-6269, fax: 202-833-7732, e-mail: education@acs.org, Internet: www.acs.org/education *The ACS Education Division serves learners and educators by building communities and providing effective chemistry education resources, grants, communities, professional development opportunities, standards and guidelines. Stop by our booth to find information that can support your efforts to provide innovative, relevant, and effective chemistry education from kindergarten through professional education.* **725**

ACS Green Chemistry Institute, 1155 16th Street, NW, Washington, DC, United States 20036, 202-872-6102, fax: 202-776-8009, e-mail: gci@acs.org, Internet: www.acs.org/gci *The ACS Green Chemistry Institute® believes that innovation in sustainable and green chemistry and engineering (GC&E) is vital to solving environmental and human health challenges. Our mission is to catalyze and enable the implementation of GC&E throughout the global chemical enterprise and empower you to re-imagine a sustainable future.* **724**

ACS Meetings & Expositions, 1155 Sixteenth Street NW, Washington, DC, United States 20036, 800-227-5558, fax: 202-872-6128, e-mail: m_stevenson@acs.org, Internet: www.acs.org/meetings *The ACS Meetings booth displays information on current and future regional meetings and the spring and fall National Meetings. Register for a regional meeting or get information on submitting an abstract to a meeting in your region. The programming is diverse and exciting! Meet the volunteers who are planning these meetings at the booth. Visit the regional meetings website at www.acs.org/regionalmeetings for a tour of this year's conferences. Information on future national meetings will be on display.* **725**

ACS Member Insurance Program, 1155 16th Street, N.W., Washington, DC, United States 20036, 800-227-5558, ext. 6037, fax: 202-872-4435, e-mail: memins@acs.org, Internet: www.acs.org/insurance *The ACS Member Insurance Program is committed to offering quality comprehensive insurance plans to members and their families. Stop by the ACS station to learn more about the plans available such as Life and Health Insurance, Auto & Homeowners, Long Term Care, Professional Liability, Chemical Educators Legal Liability and more.* **725**

ACS Membership, 1155 16th St., NW, Suite OTH420, Washington, DC, United States 20036, 2028726062, Internet: www.acs.org/MemberHandbook *Visit Membership in the ACS Booth to pick up a copy of the 2017 Member Handbook and a booth raffle card. Visit at least 5 ACS Kiosks and return your completed card to be entered to win one of 10 prizes!* **725**

ACS Publications, 1155 16th Street, N.W., Washington, DC, United States 20036, 202-872-6862, fax: 202-872-6005, e-mail: s_jackson@acs.org, Internet: pubs.acs.org *ACS Publications is the leading publisher in chemistry and related sciences. Stop by our booth to receive free gifts and information on our newest journal, ACS Earth and Space Chemistry, and be sure to participate in our interactive author mosaic by using the hashtag #ACSmosaic. Visit ACS theater to meet Priestley Medalist Tobin Marks and learn about C&EN's Molecule of the Moment.* **725**

ACS Store, 1155 16th Street, NWWashington, DC 20036, United States, Phone: 800-ACS-5558 Fax: 202-872-6067, Internet: http://www.acs.org/store **725**

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US EPA Green Chemistry Program, 1200 Pennsylvania Avenue, Mail Code 7406M, Washington, DC, United States 20460, Internet: www.epa.gov/greenchemistry *The U.S. EPA Green Chemistry Program is a voluntary, partnership program whose mission is to promote innovative chemical technologies that reduce or eliminate the use or generation of hazardous substances in the design, manufacture, and use of chemical products and processes. The Program accomplishes these goals through multiple activities including: The Presidential Green Chemistry Challenge Awards; designing tools, databases, and educational materials; and supporting research through grants and fellowships.* **728**

V&P Scientific, Inc., 9823 Pacific Heights Blvd., Suite T, San Diego, CA, United States 92121, 858-455-0643, fax: 858-455-0703, e-mail: sales@vp-scientific.com, Internet: www.vp-scientific.com **213**

Vacuubrand, 11 Bokum Road, Essex, CT, United States 06426, 860-767-2562 ext. 125, fax: 860-767-2563, Internet: www.vacuubrand.com *VACUUBRAND offers exceptionally quiet, corrosion-resistant, oil-free vacuum pumps with ultra-long service intervals for labs, scale-up and OEM use. Products include both simple dry pumps and self-regulating, automated vacuum systems for critical evaporative applications. The line also includes the unique HYBRID pumps, which reduce oil-changes by 90%, even in corrosive applications. VACUUBRAND will also show corrosion-resistant digital vacuum gauges and controllers. New products include high flow-rate, chemical-resistant dry vacuum pumps for kilo-lab and pilot-scale applications.* **1519**

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Vacuum Process Engineering, Inc., 110 Commerce Circle, Sacramento, CA 95815, United States, 916-925-6110, Internet: http://www.vpei.com 1906

Vacuum Technology Inc., 15 Great Republic Drive, Unit #4, Gloucester, MA, United States 01930, 978-879 4302, fax: 978-879 4387, e-mail: sam.cai@vti-glovebox.com, Internet: www.vti-glovebox.com *Based in Gloucester, Massachusetts, Vacuum Technology Inc. builds and services the glove box needs of educational and industrial clients worldwide by integrating best–in-class components sourced from Europe, Asia, UK and the USA. Along with standard offerings, we proudly highlight our engineering talent and customer-centric customization shop.* **1814**

Vapourtec Ltd., Unit 16, Park Farm Business Centre, Fornham St Genevieve, Suffolk IP28 6TS, United Kingdom, 44 1284 728659, fax: 44 1284 728352, e-mail: duncan.guthrie@vapourtec.com, Internet: http://www.vapourtec.com *Vapourtec manufacture two series of flow chemistry systems:*
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Vigor Tech USA, LLC, 5100 Westheimer Road, Suite 200, Houston, TX, United States 77056, 716 200 1200, e-mail: info@vigor-glovebox.com, Internet: www.vigor-glovebox.com *Vigor Tech USA is a leading international producer of gloveboxes, purification systems and other inert atmosphere equipment. Vigor provides its customers with the most reliable, affordable and innovative inert workstations on the market, with a special focus on custom glovebox projects and instrument integrations.* **1300**

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Waters Corp., 34 Maple Street, Milford, MA, United States 01757, 508-482-2000, fax: 508-482-2674, e-mail: info@waters.com, Internet: www.waters.com *Waters Corporation, the premium brand in the analytical instruments industry, creates business advantages for laboratory-dependent organizations by delivering practical and sustainable scientific innovation to enable significant advancements in chemical analysis, healthcare delivery, environmental management, food safety, and water quality worldwide.* **609**

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Welch by Gardner Denver, 1601 Feehanville Drive, Suite 550, Mount Prospect, IL, United States 60056, 847-676-8800, fax: 847-677-8606, Internet: www.welchvacuum.com **1200**

Westcoast Separation, LLC, 3201 Corte Malpaso, #310, Camarillo, CA, United States 93012, 805-504-7767, Internet: www.westcoastseparations.com *Westcoast Separations specializes in chromatographic technologies for method development, analysis and purification of small molecules. We offer screening of columns, method development and purification for chiral and achiral molecules. We combine the benefits of analytical and preparative HPLC and Supercritical Fluid Chromatography (SFC) to achieve separation goals and results.* **1632**

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APRIL 2-4, 2017

SUNDAY, 6PM - 8:30PM

MONDAY & TUESDAY, 9AM - 5PM

MOSCONE CENTER, SOUTH BLDG., HALLS B & C

GRAND HYATT SAN FRANCISCO

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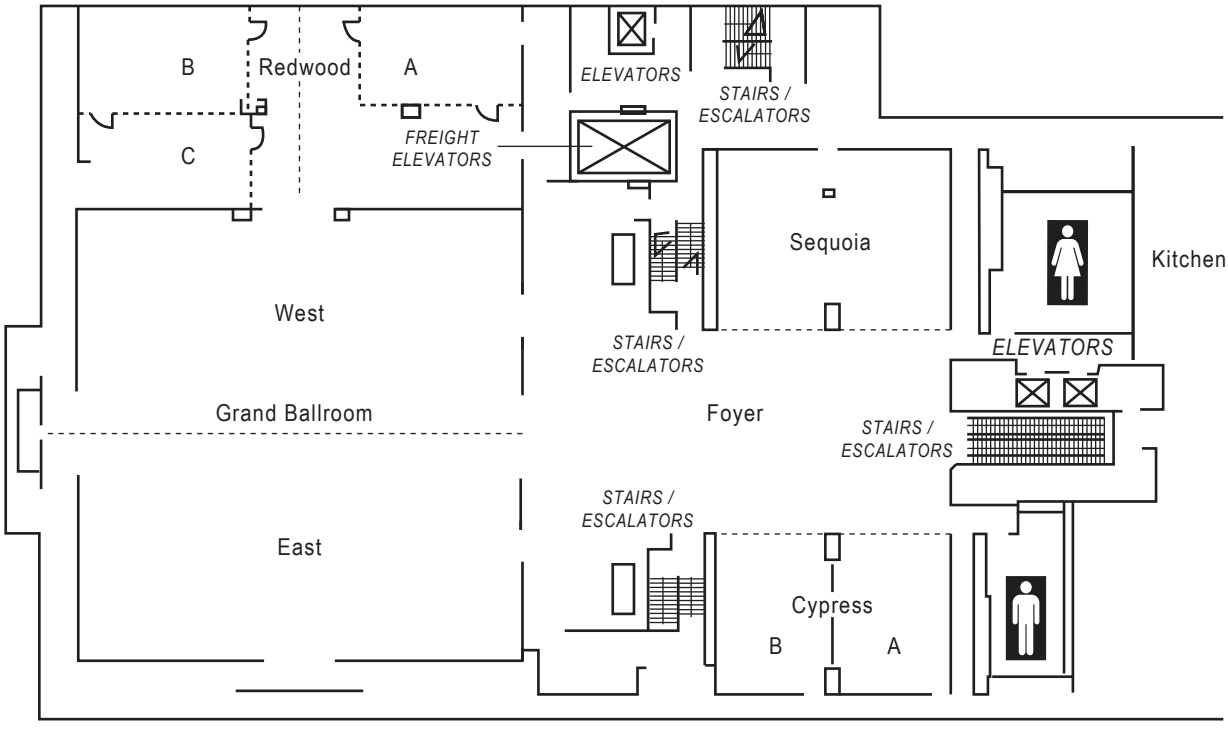
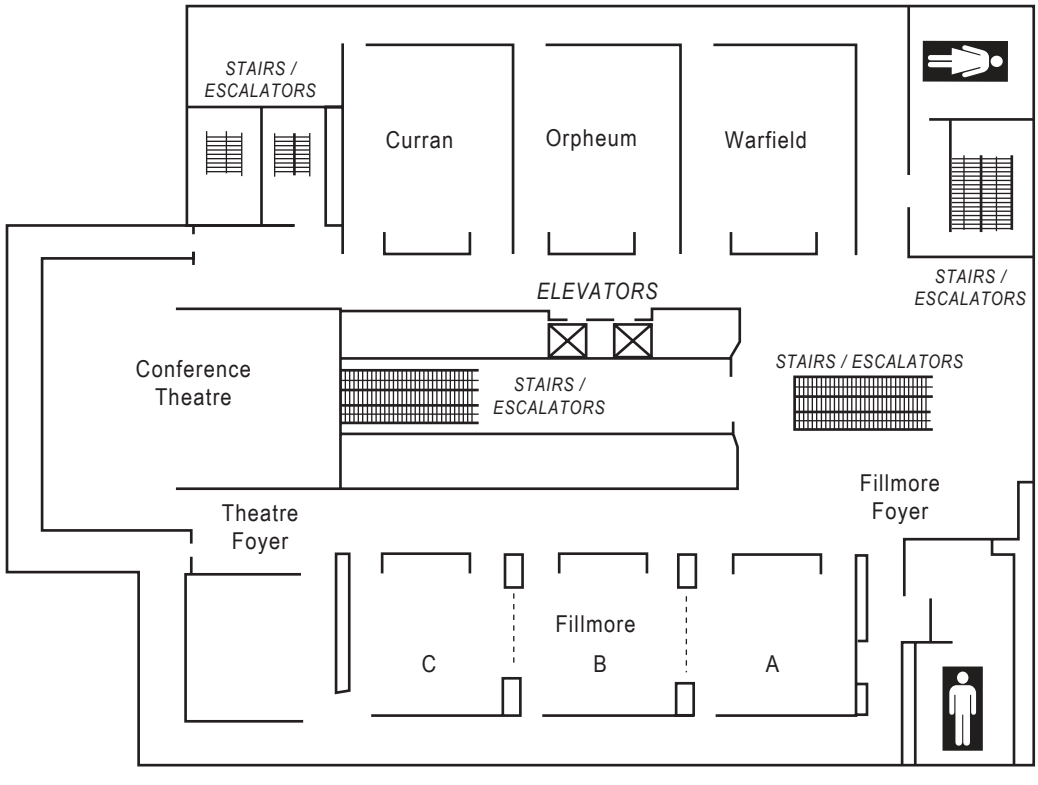
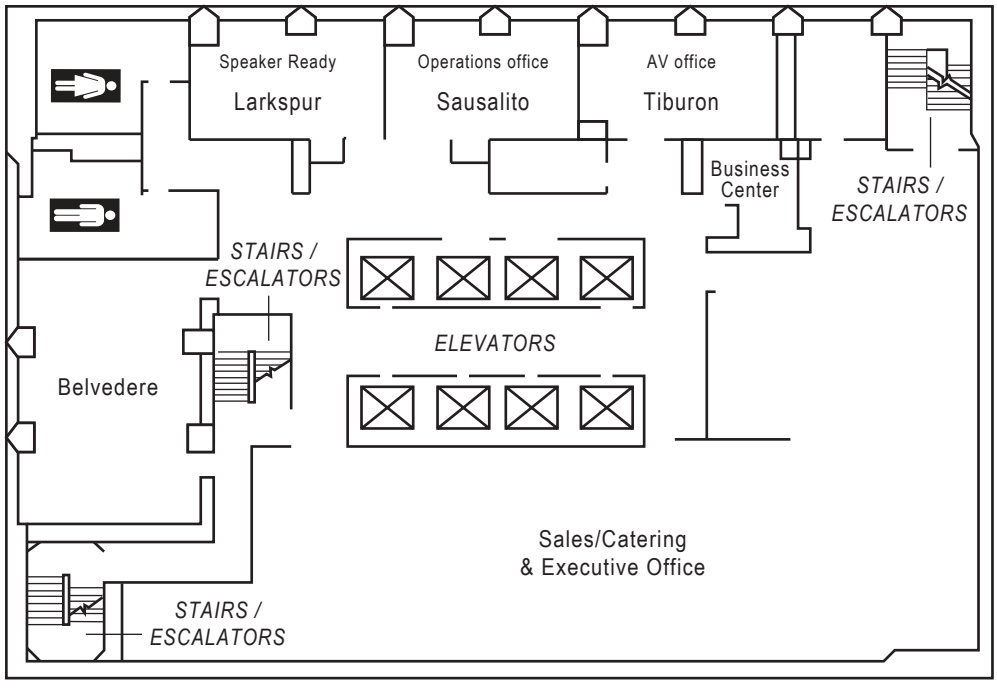


Theatre Level

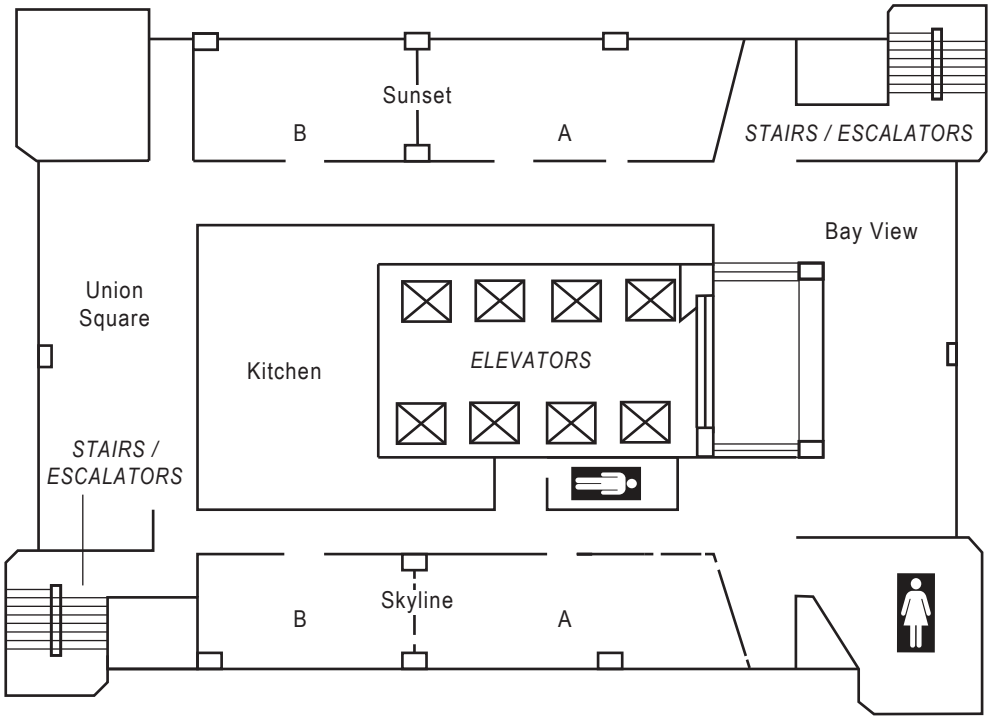


GRAND HYATT SAN FRANCISCO

Second Floor



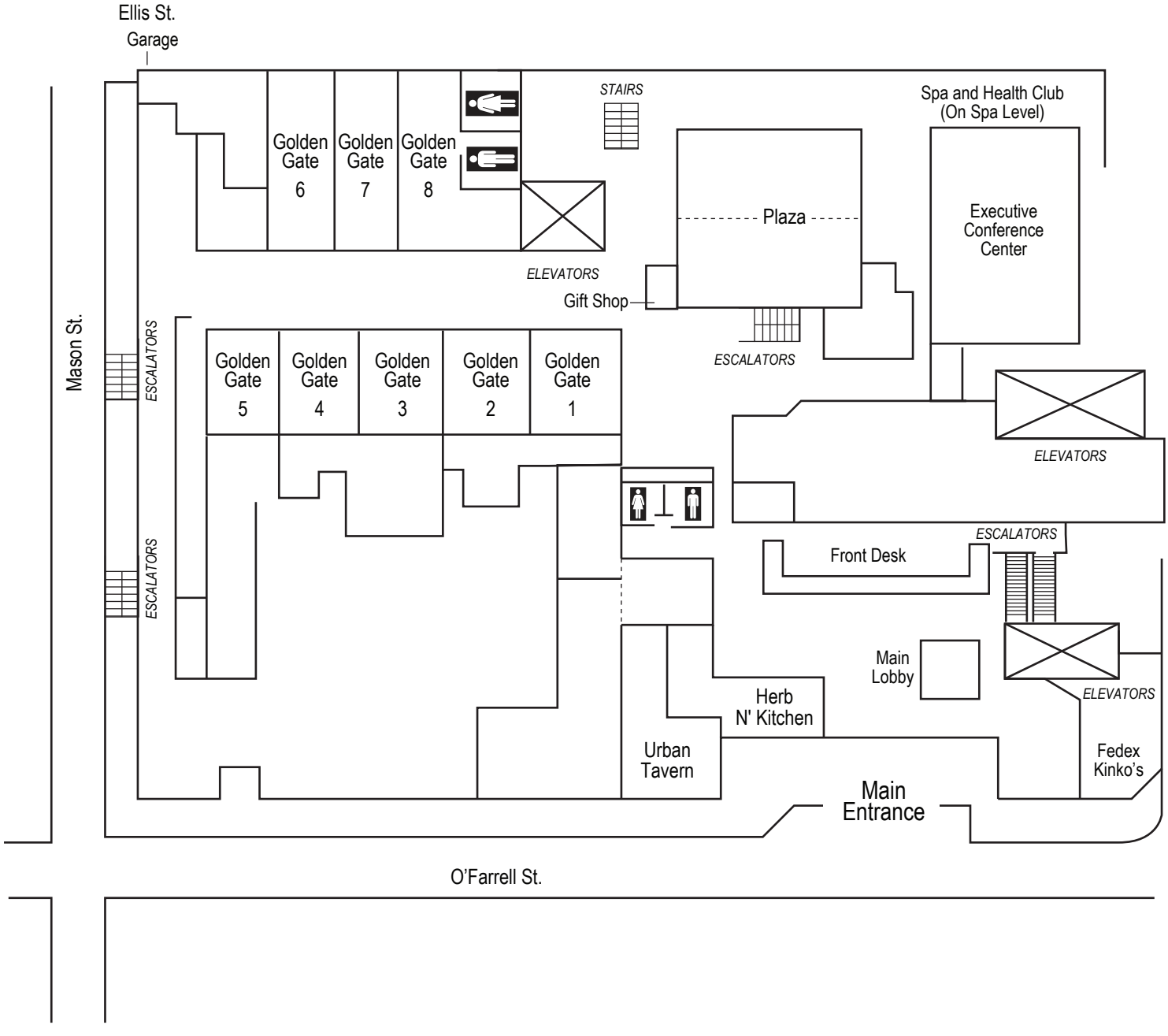
36th Floor



HILTON UNION SQUARE

Tower 3

Lobby Level



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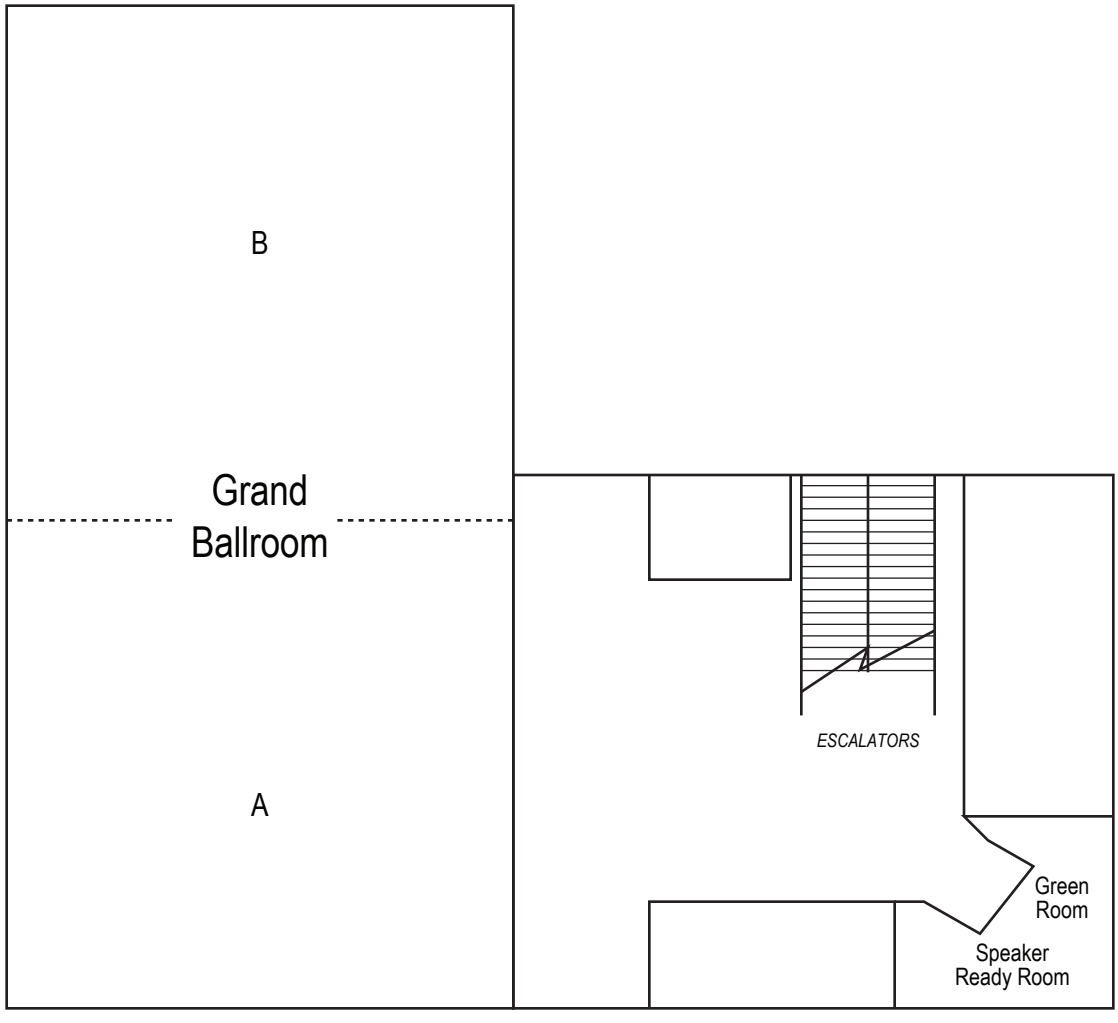
Tower 3

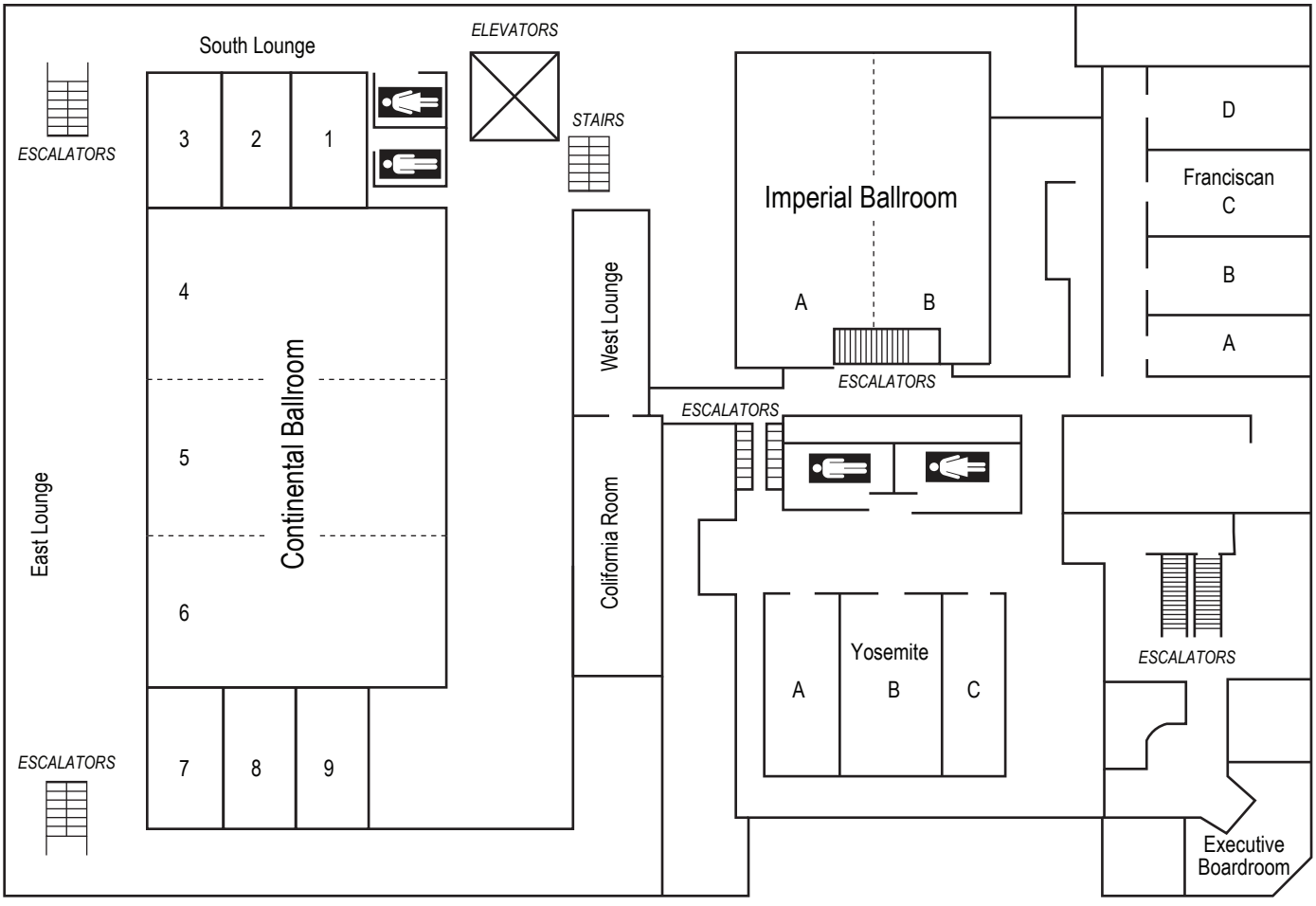
GB Level



HILTON UNION SQUARE

Tower 3

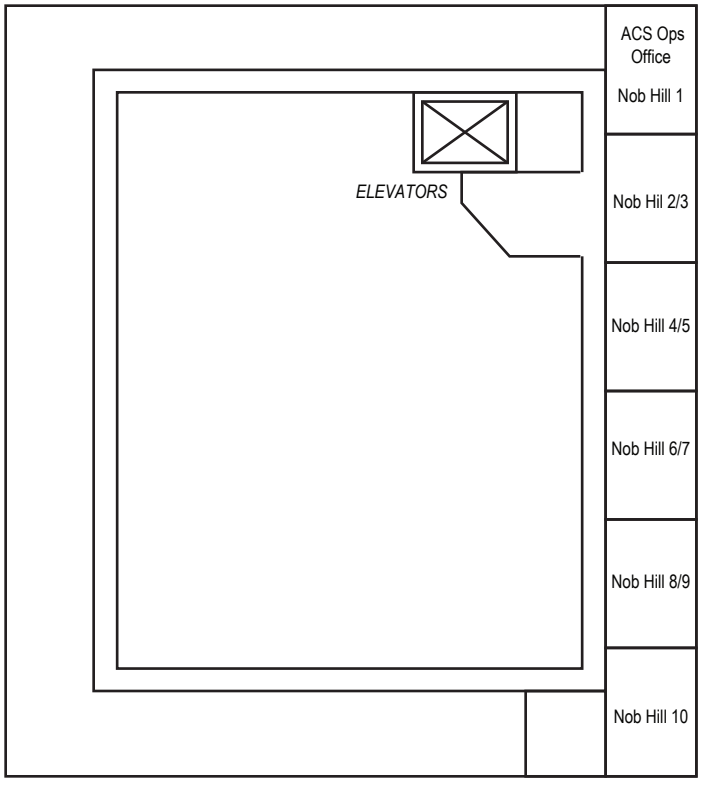
B Ballroom Level



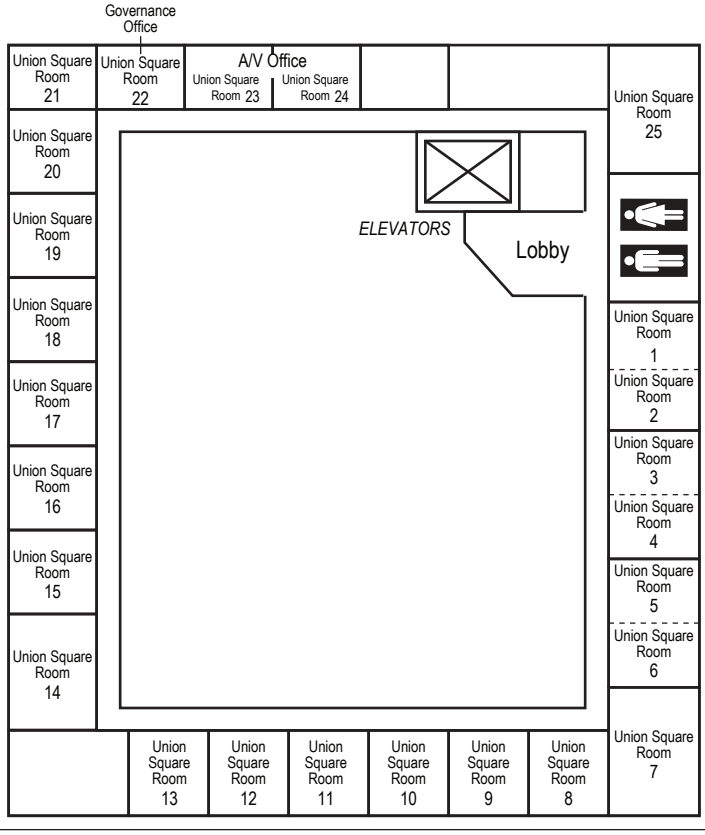
HILTON UNION SQUARE

Sixth Floor

Tower 3

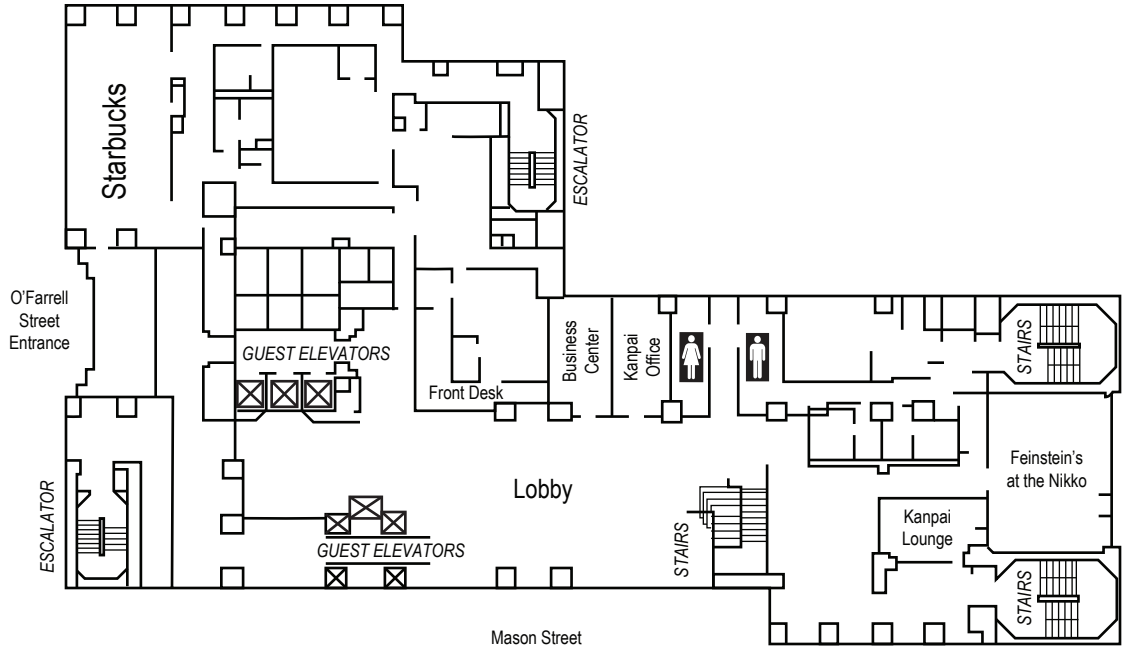


Fourth Floor

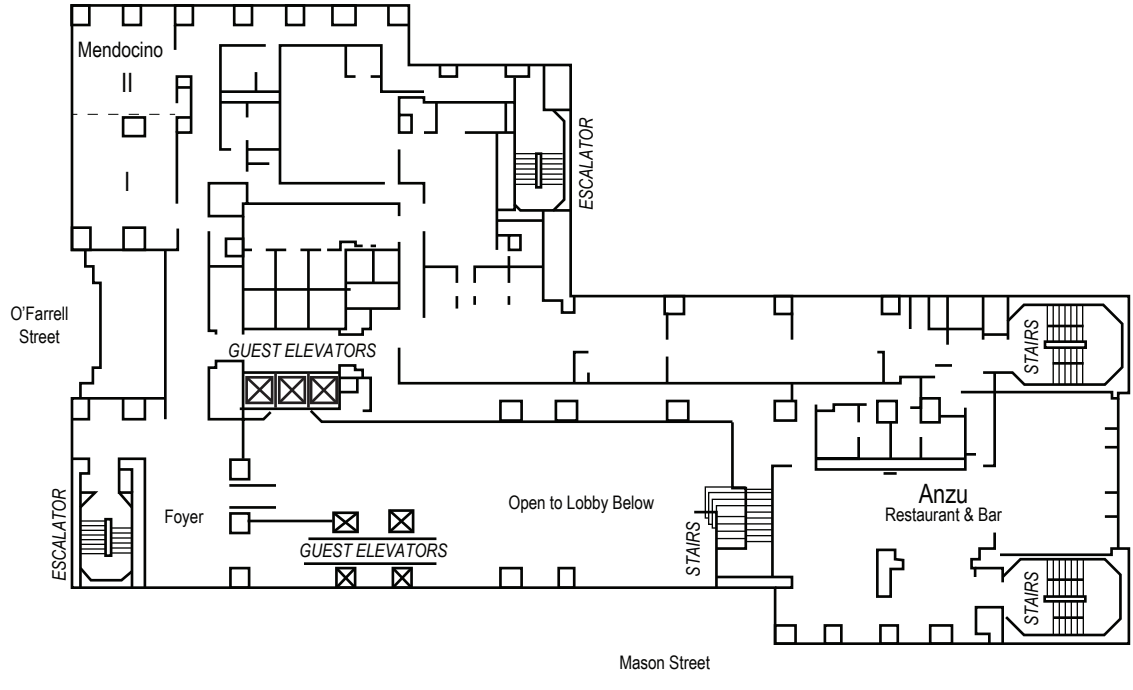


HOTEL NIKKO

First Floor

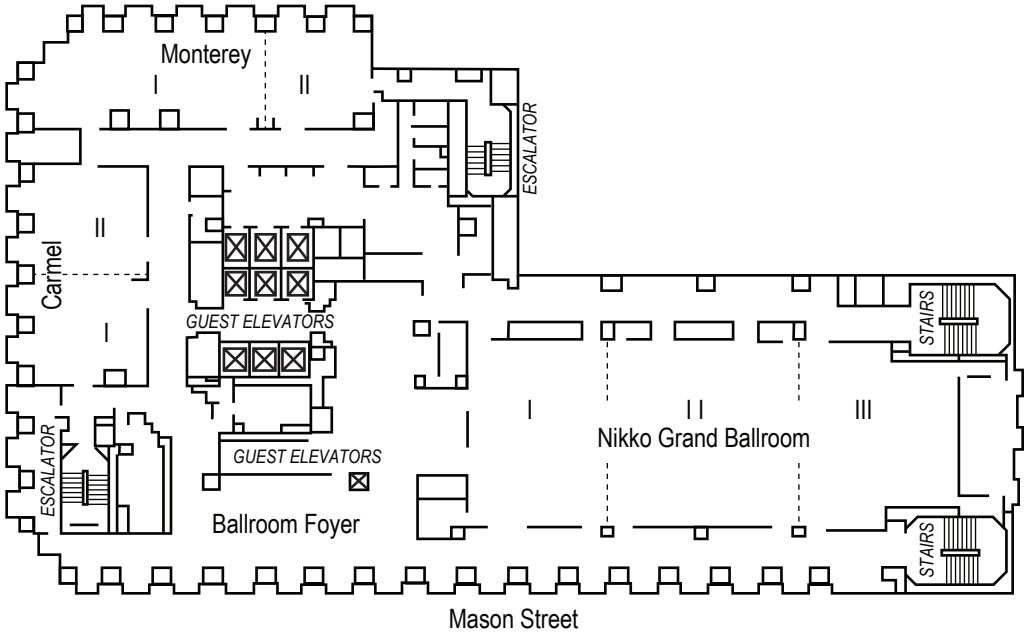


Second Floor

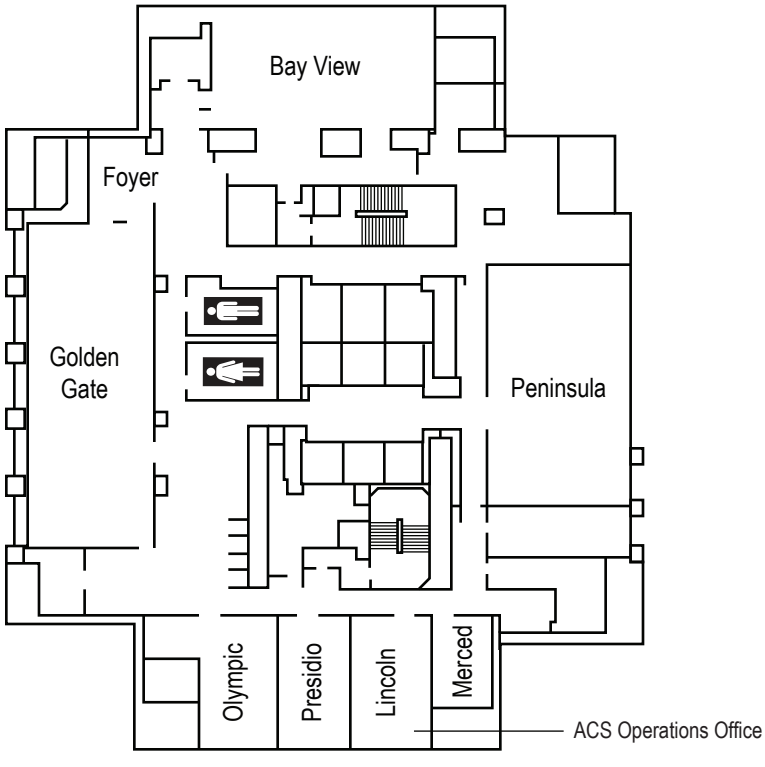


HOTEL NIKKO

Third Floor

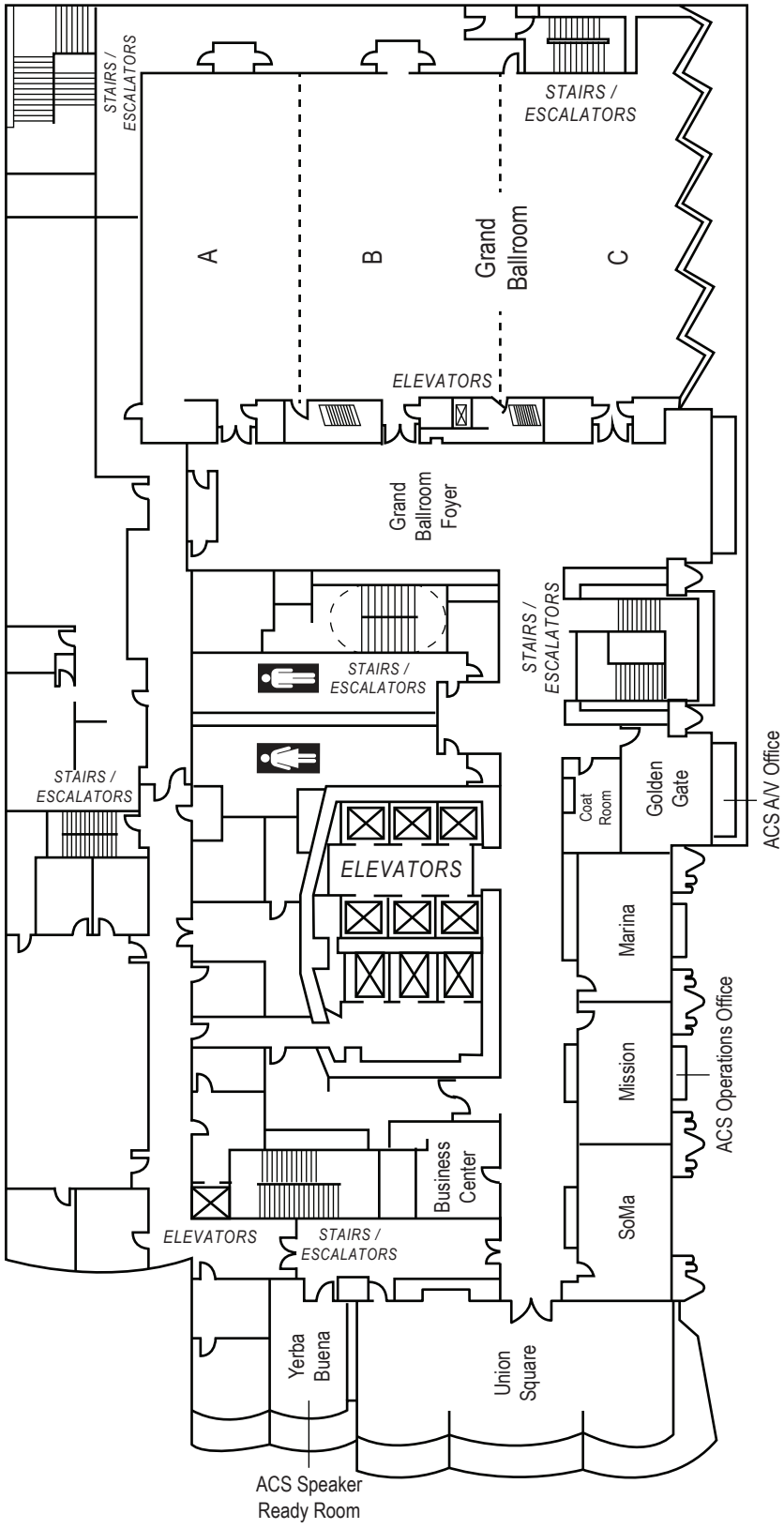


Twenty Fifth Floor



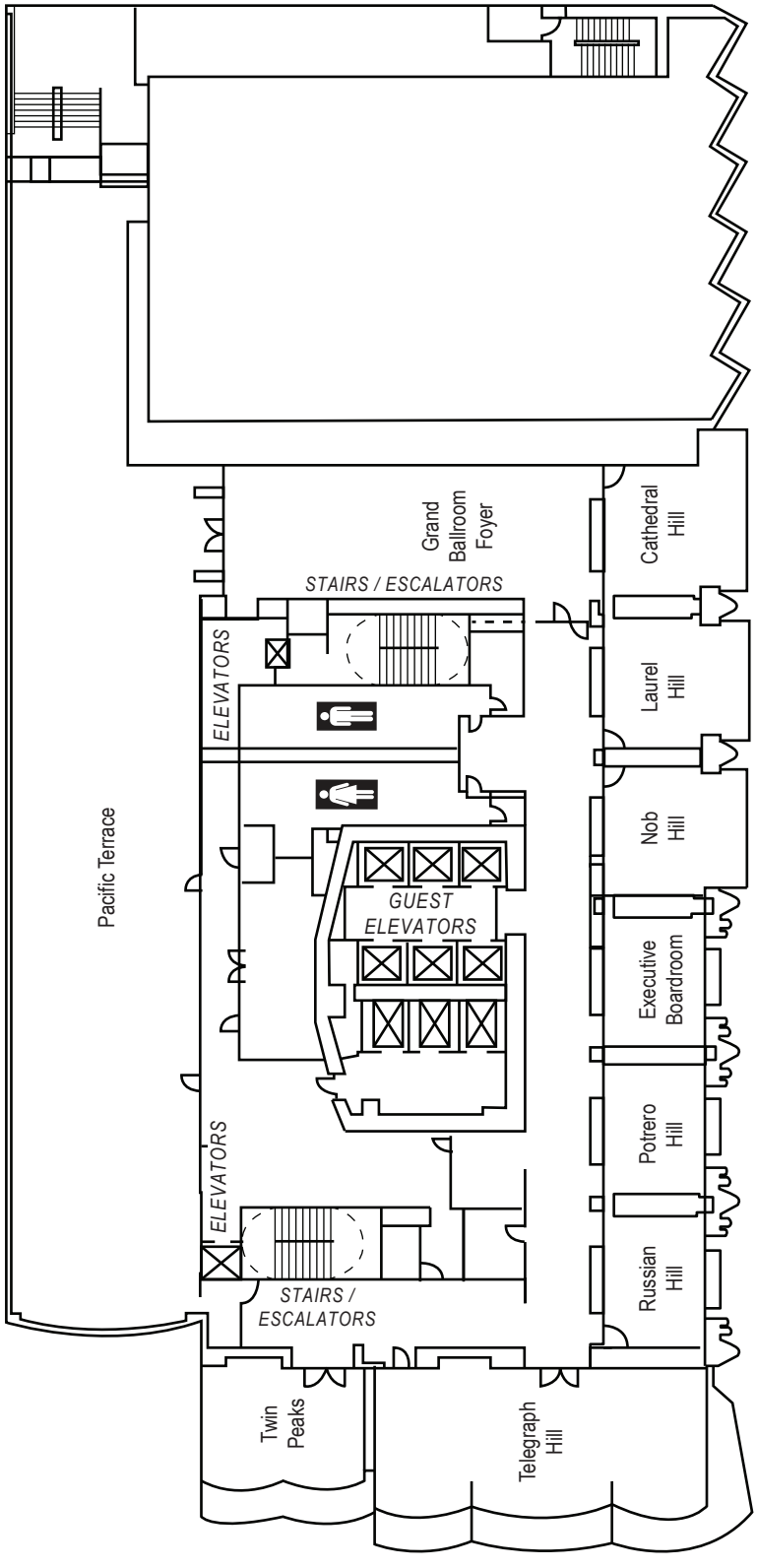
INTER CONTINENTAL

3rd Floor



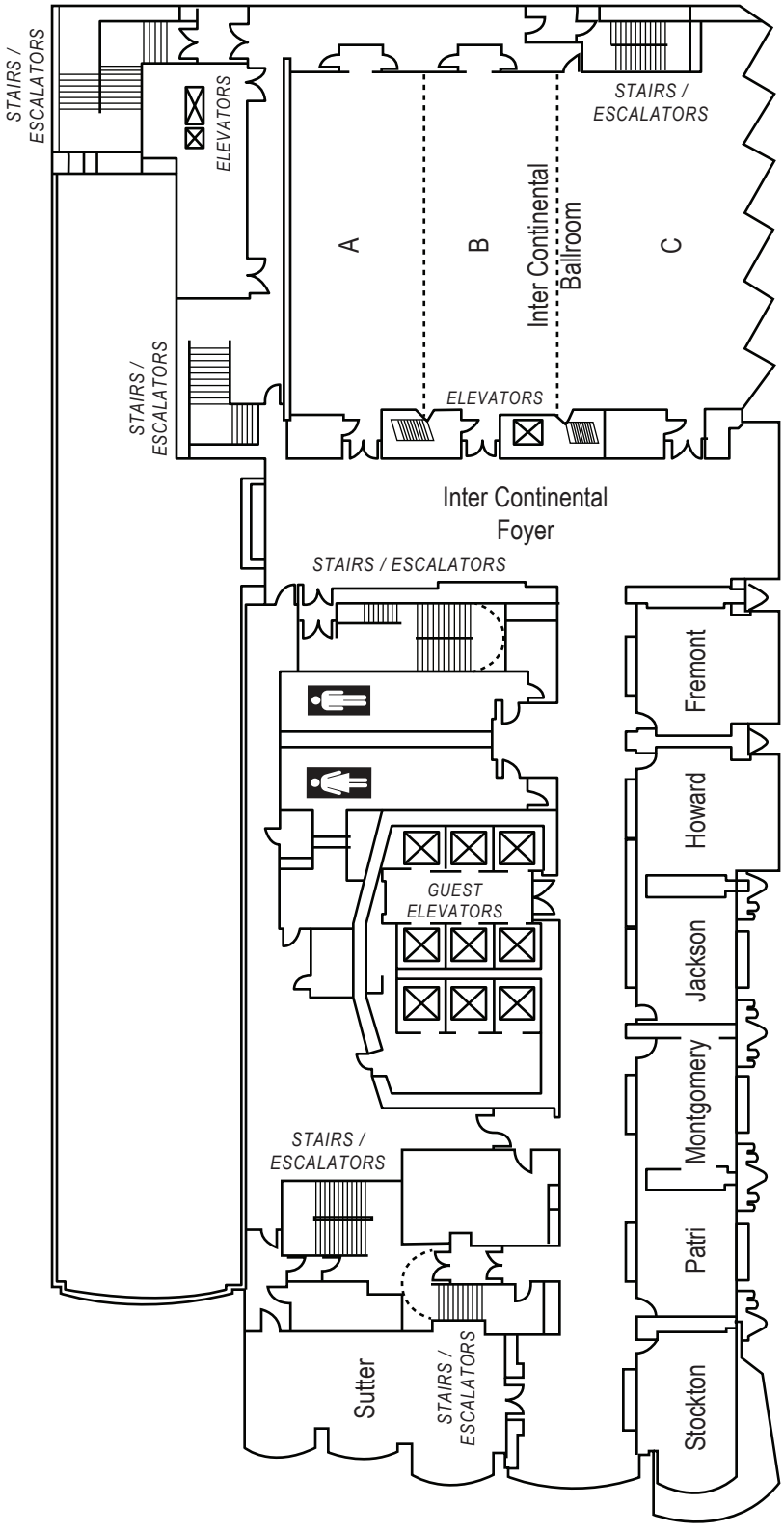
INTER CONTINENTAL

4th Floor



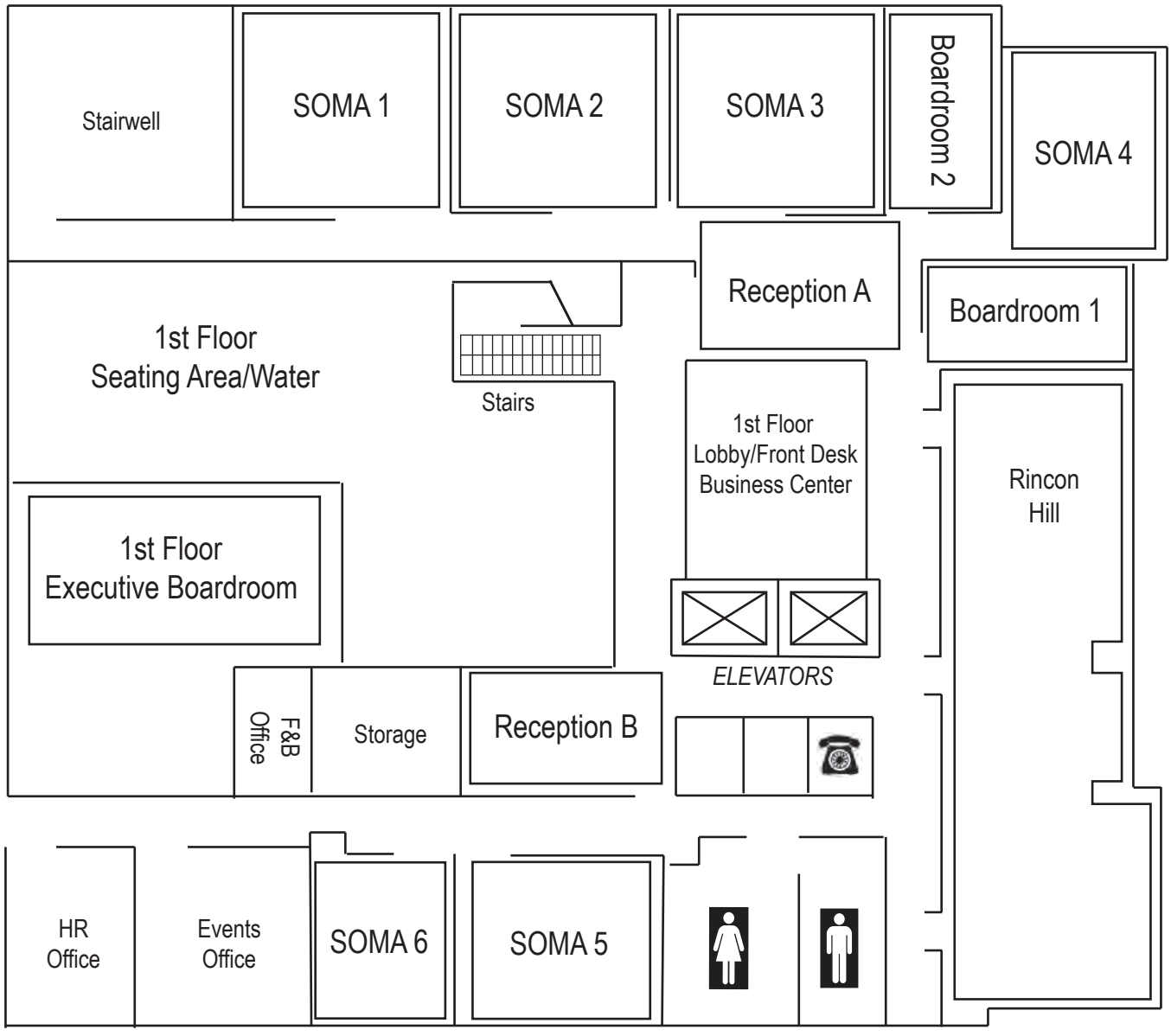
INTER CONTINENTAL

5th Floor



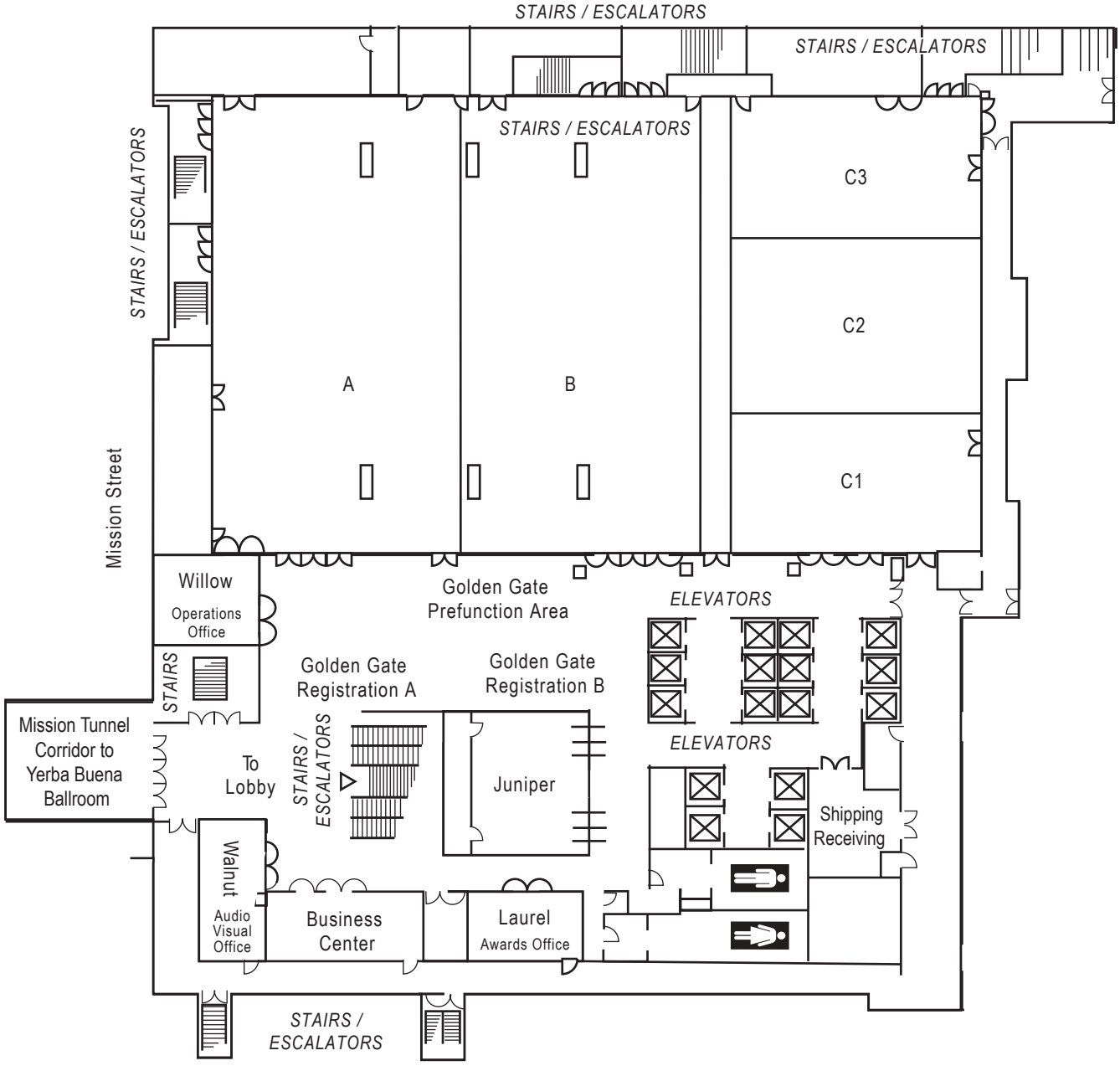
MARRIOTT COURTYARD

Meeting Rooms and Reception Areas Floor Plans



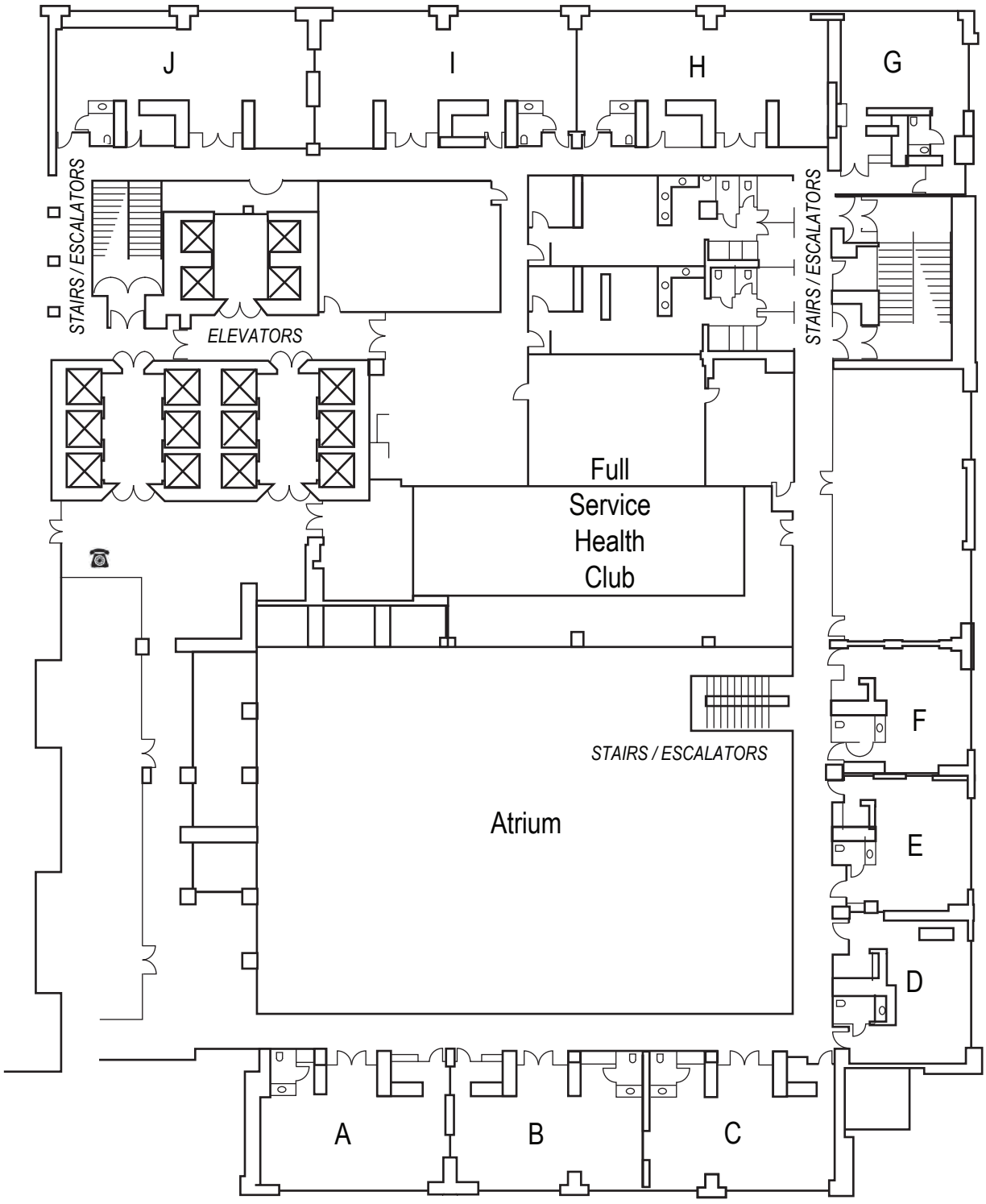
MARRIOTT MARQUIS

Golden Gate Ballroom



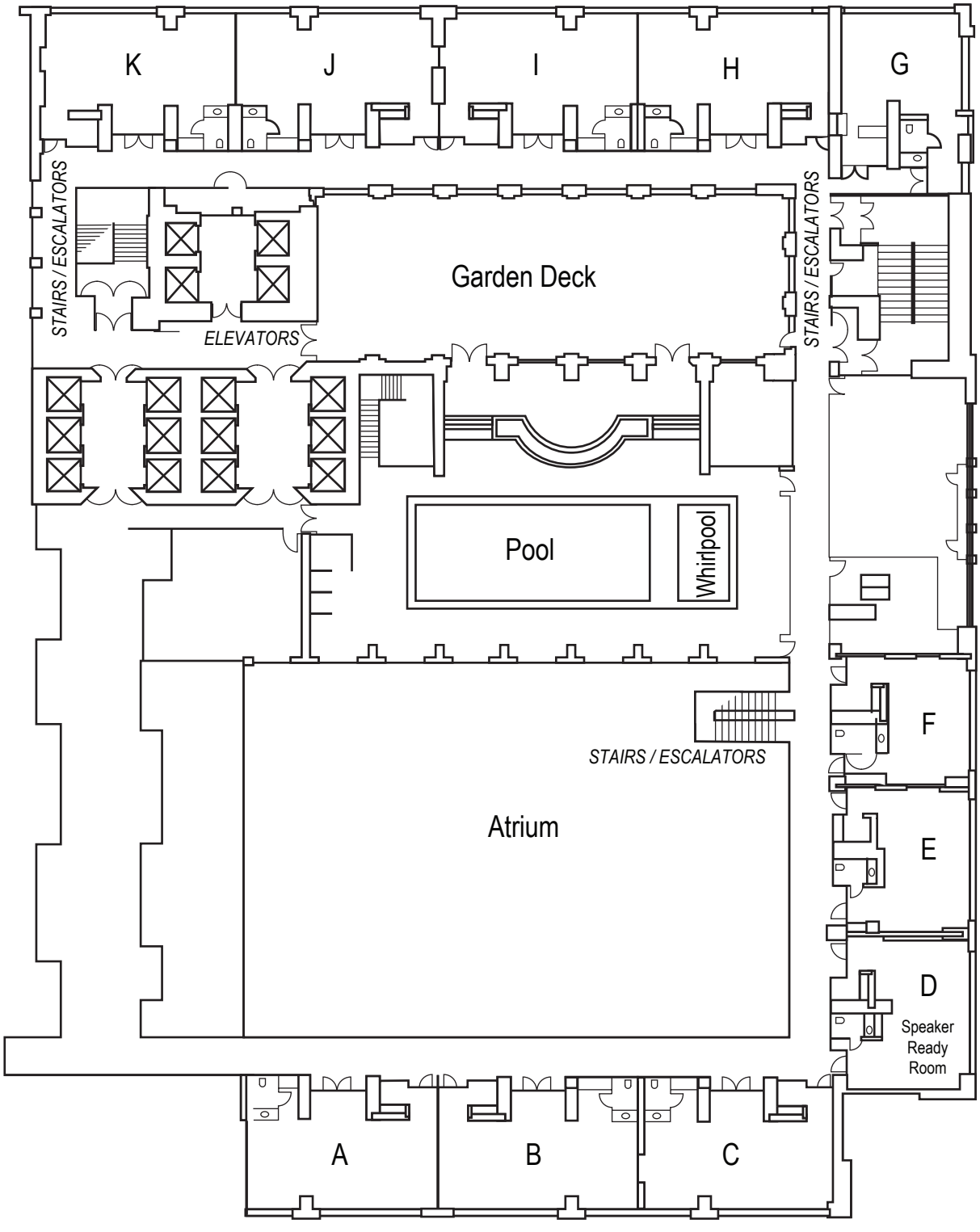
MARRIOTT MARQUIS

Pacific Fourth Floor



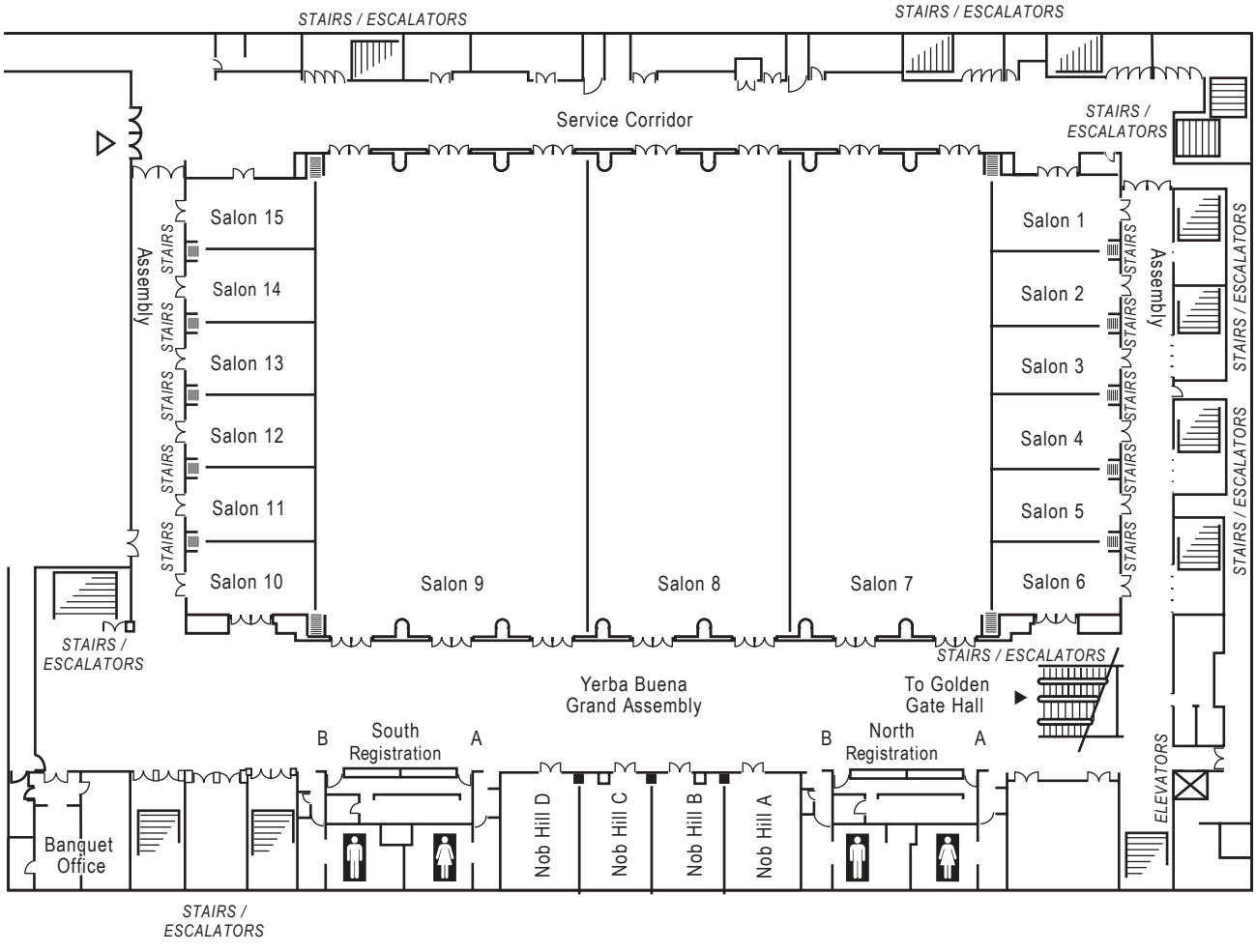
MARRIOTT MARQUIS

Sierra Fifth Floor

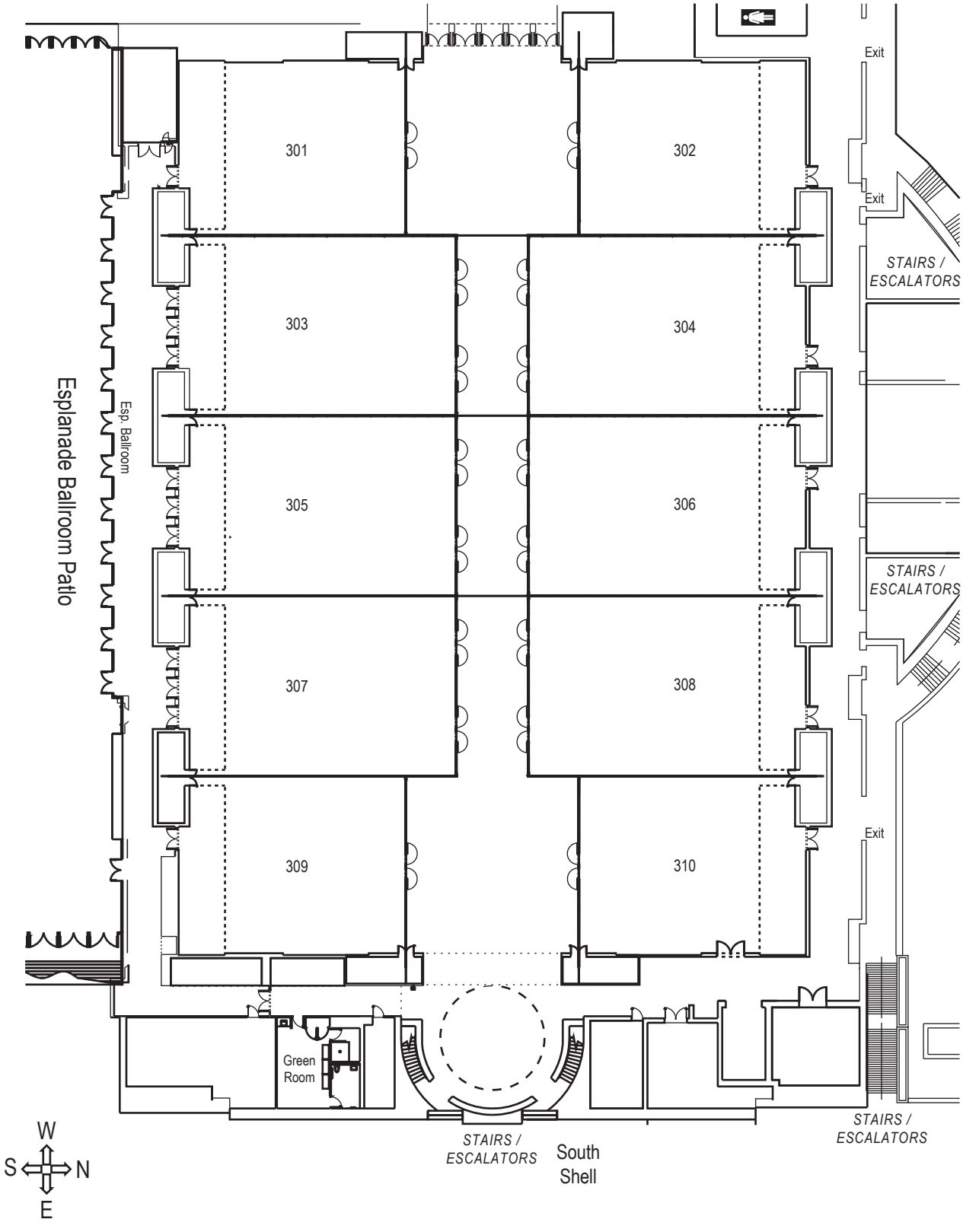


MARRIOTT MARQUIS

Yerba Buena Ballroom



MOSCONE ESPLANADE



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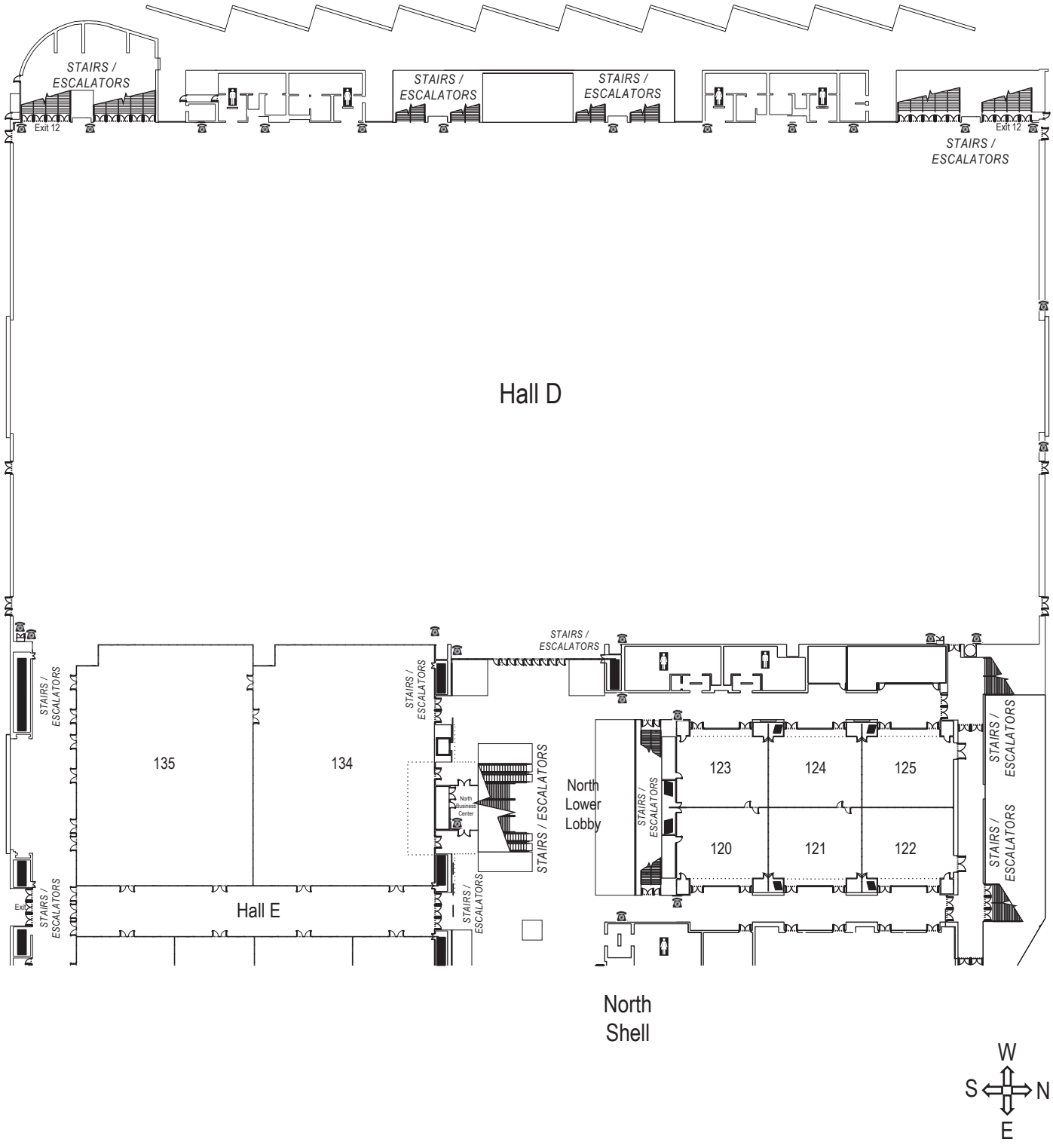
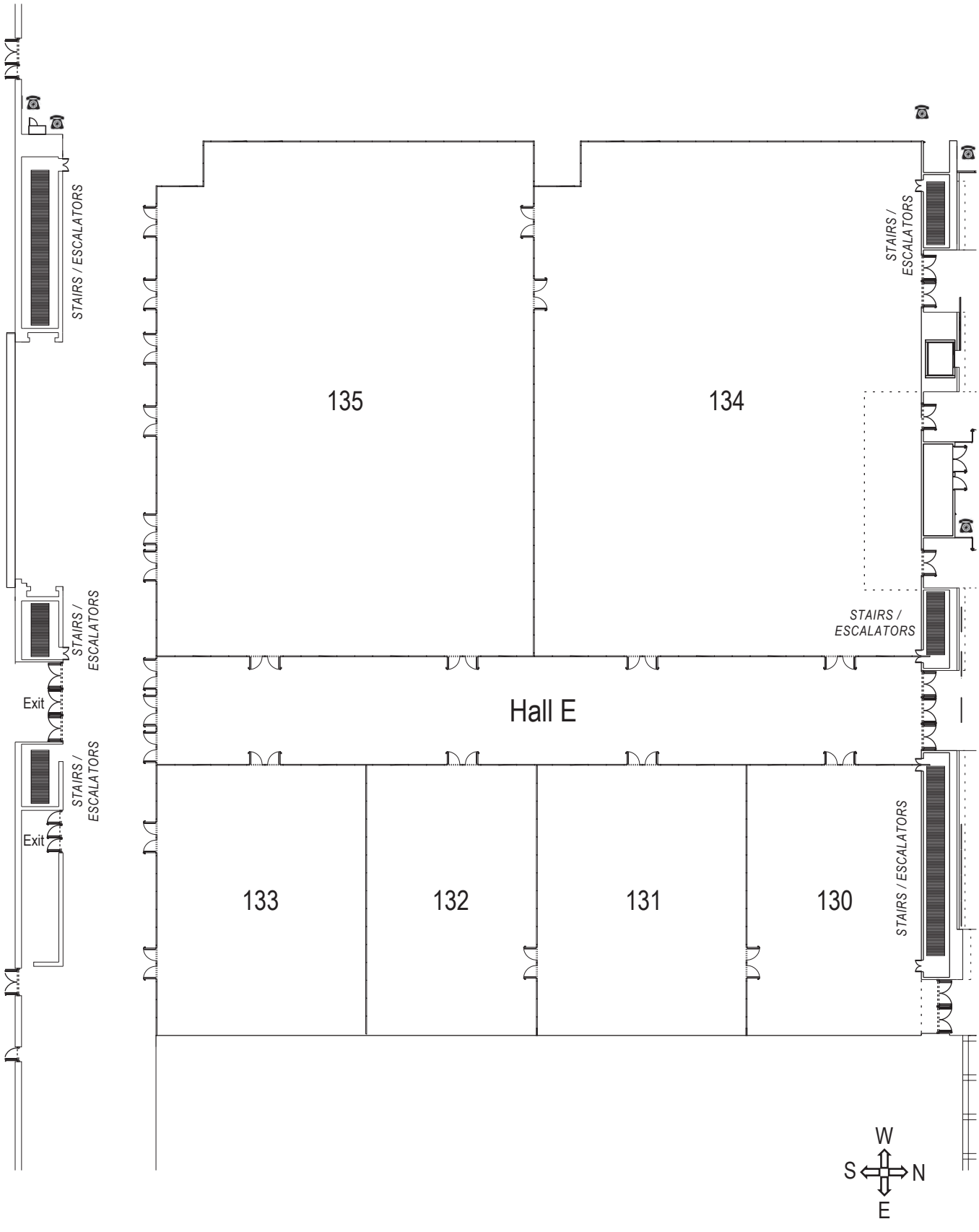
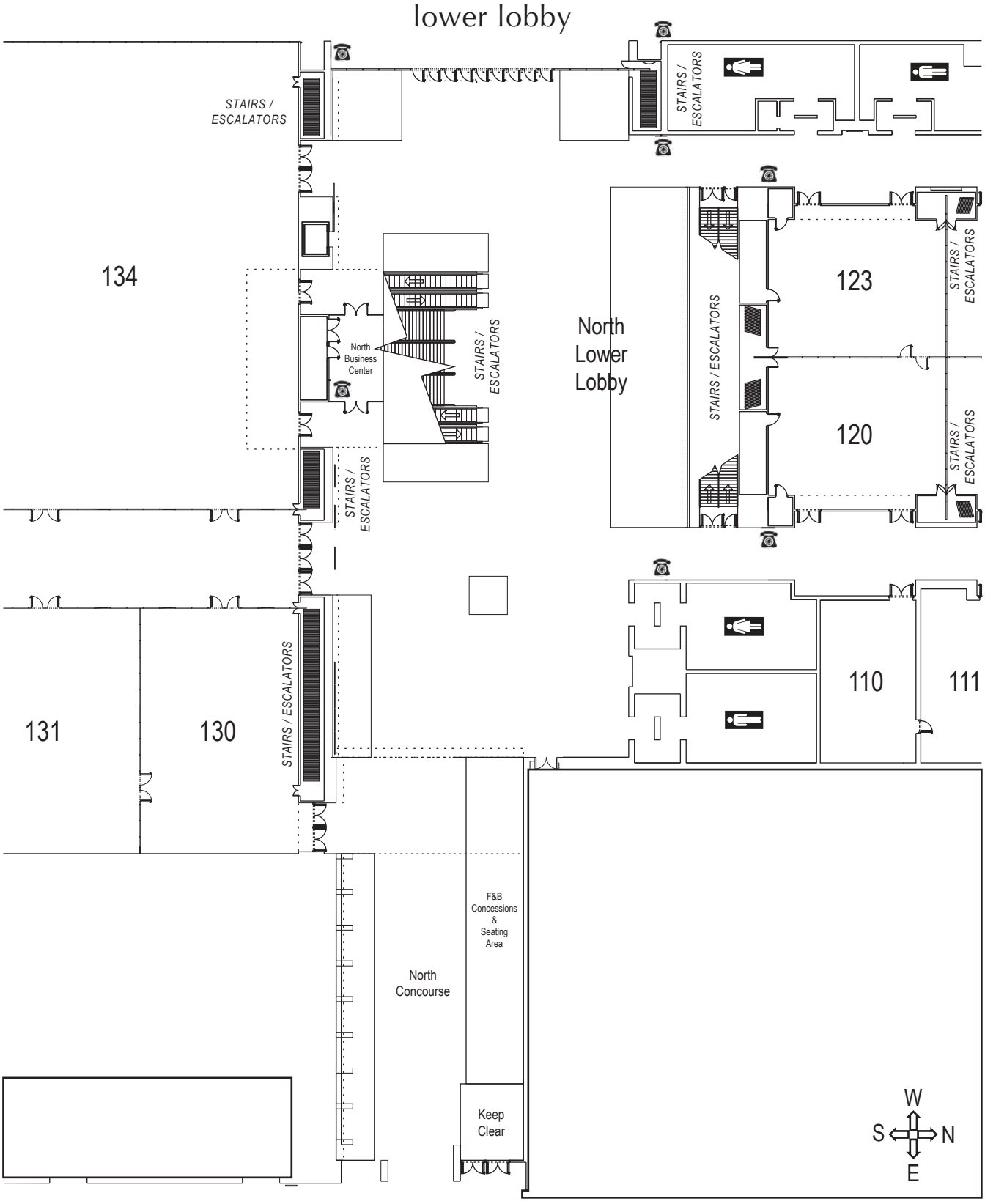


MOSCONE MEETING ROOMS 130-135



MOSCONE NORTH



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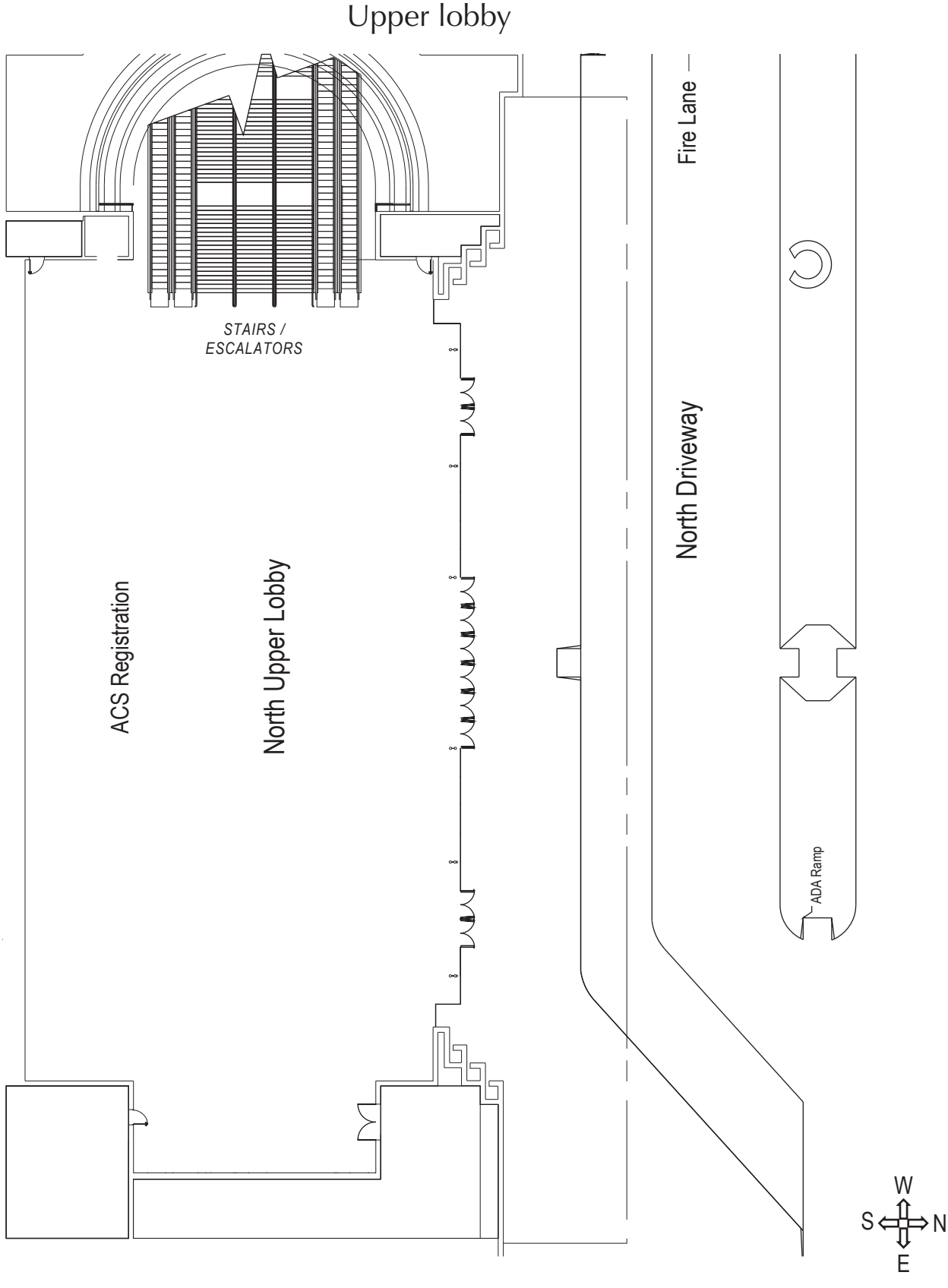
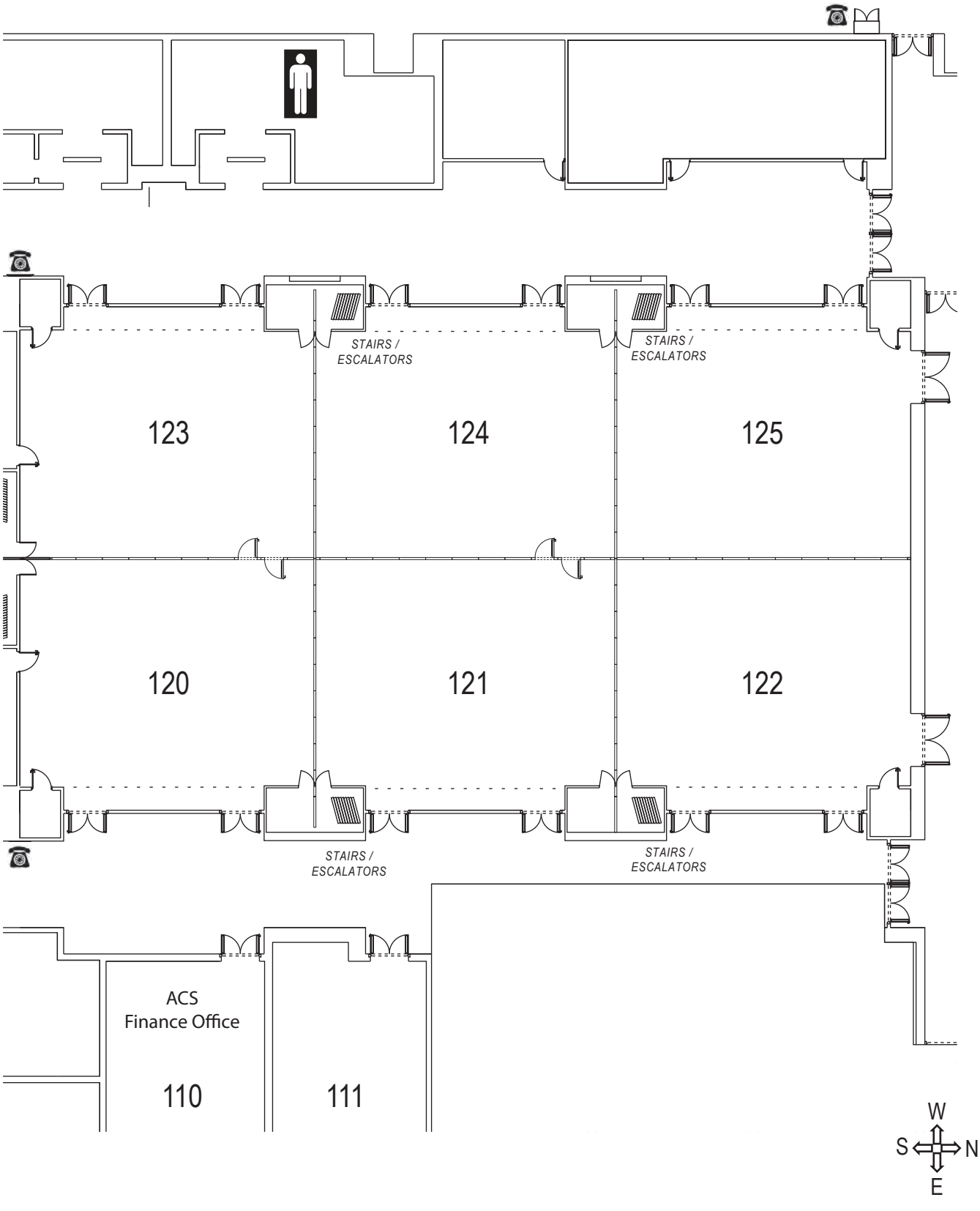
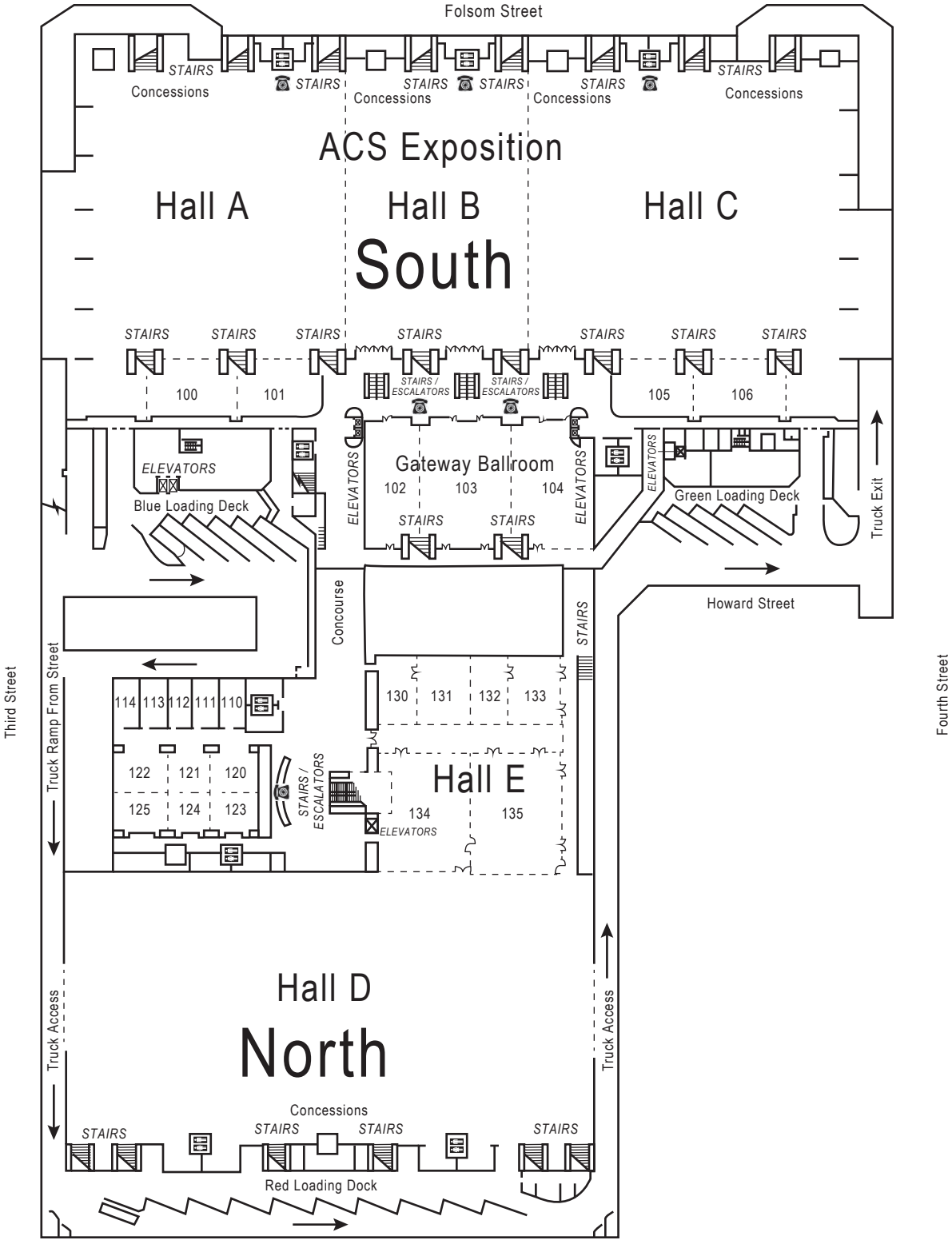


MOSCONE NORTH BLDG MEETING SPACE

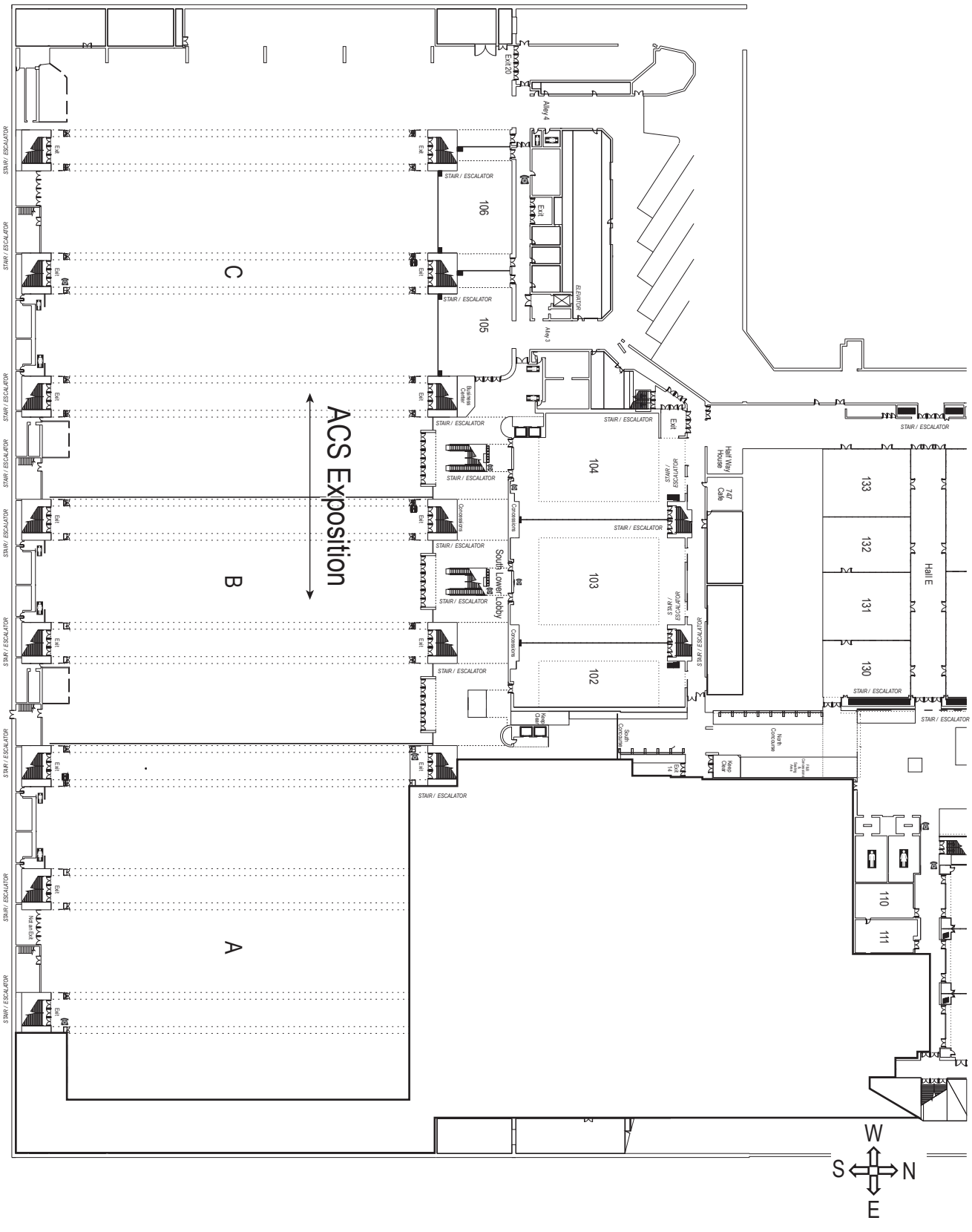


MOSCONE SOUTH & NORTH

Exhibit Level

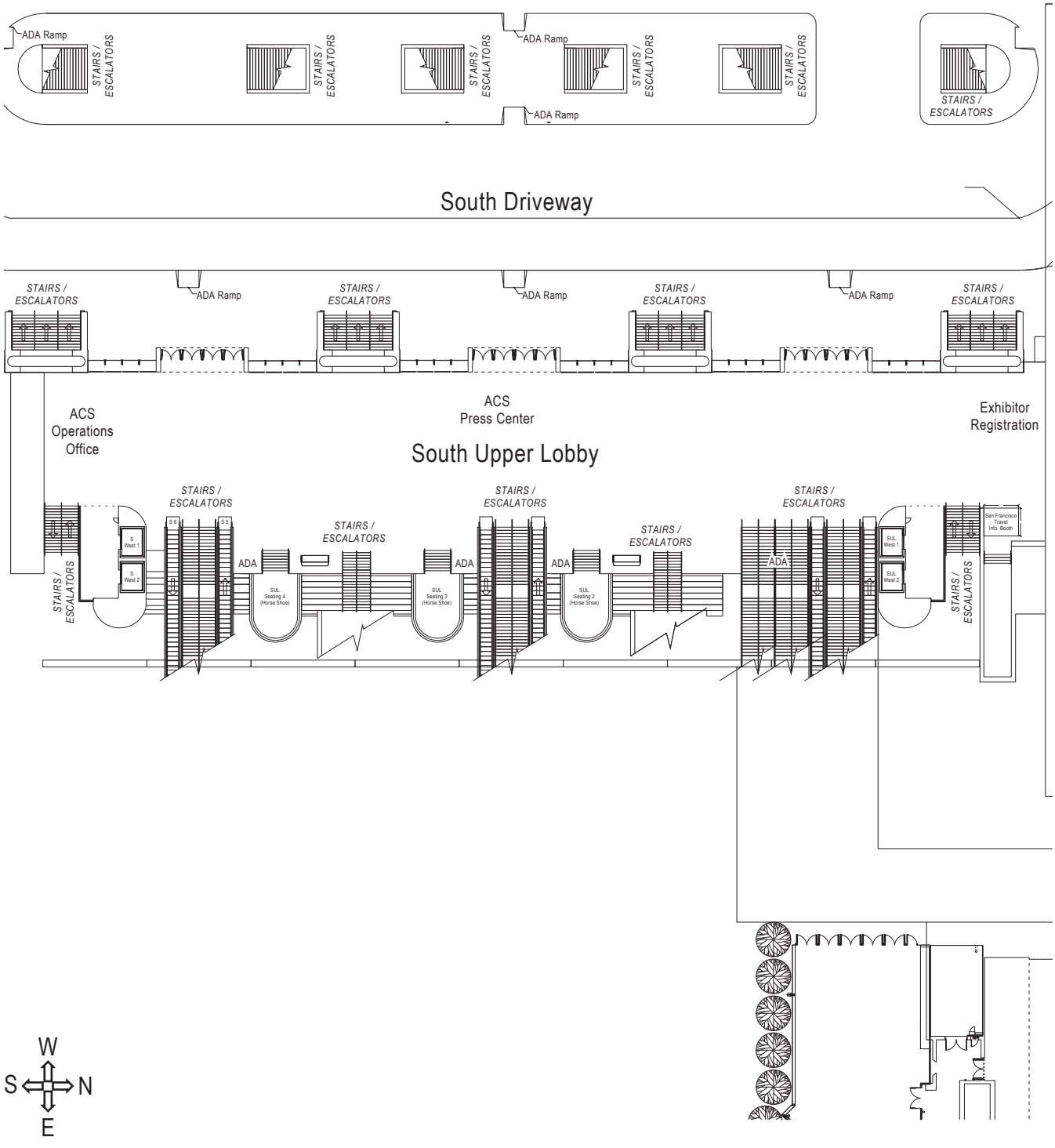


MOSCONE SOUTH BLDG HALLS A, B AND C

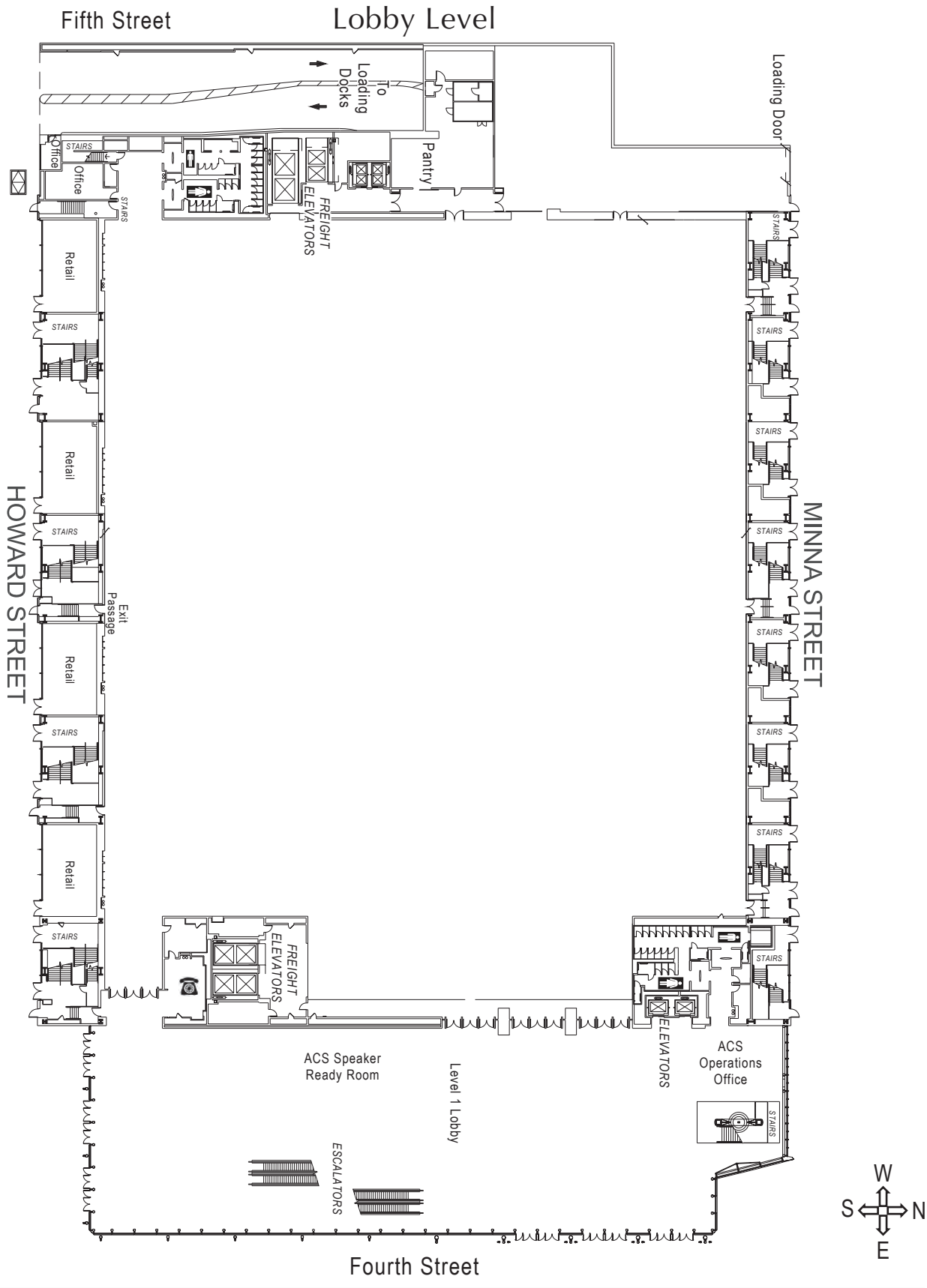


MOSCONE SOUTH

Upper Lobby

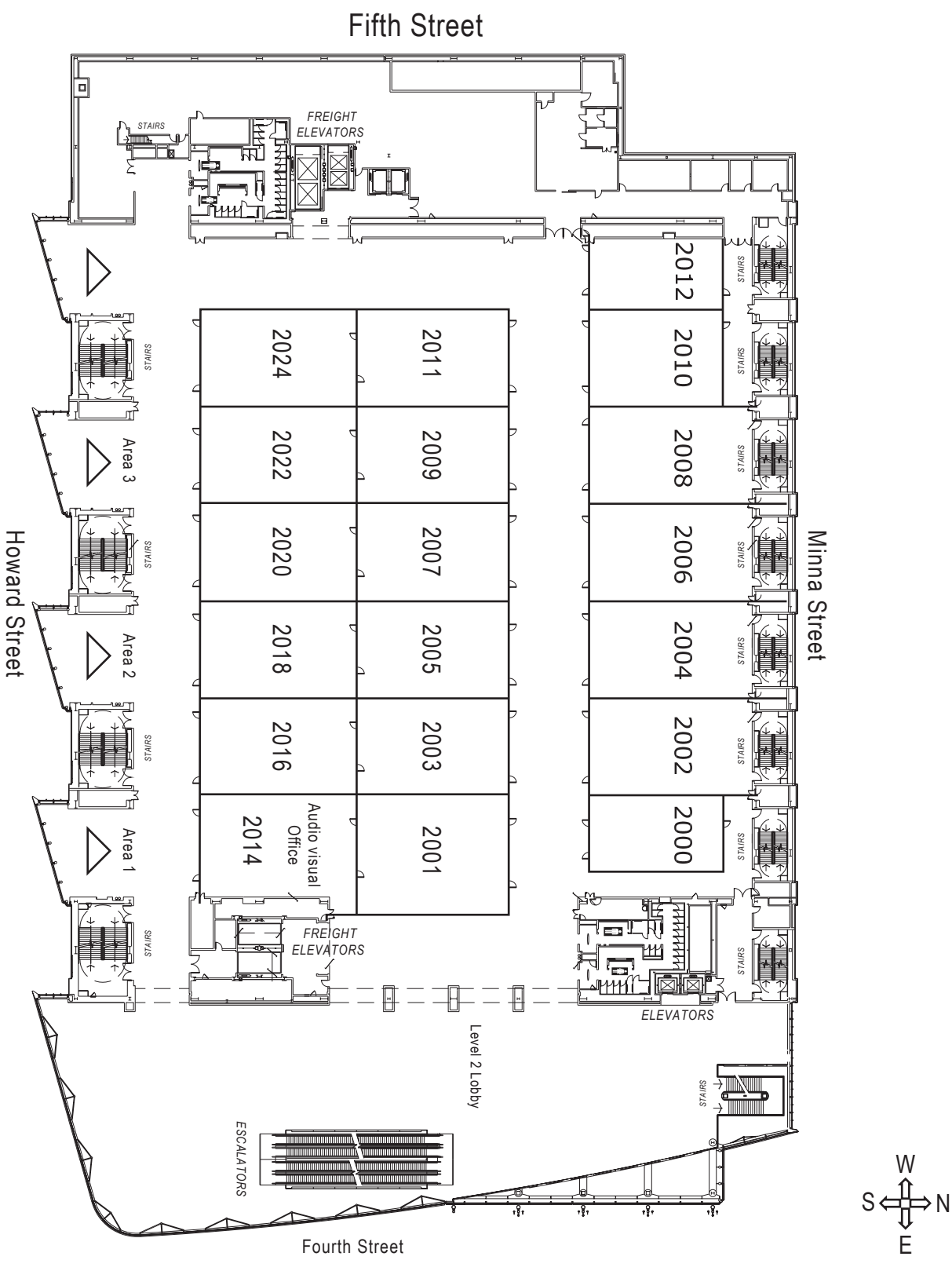


MOSCONE WEST



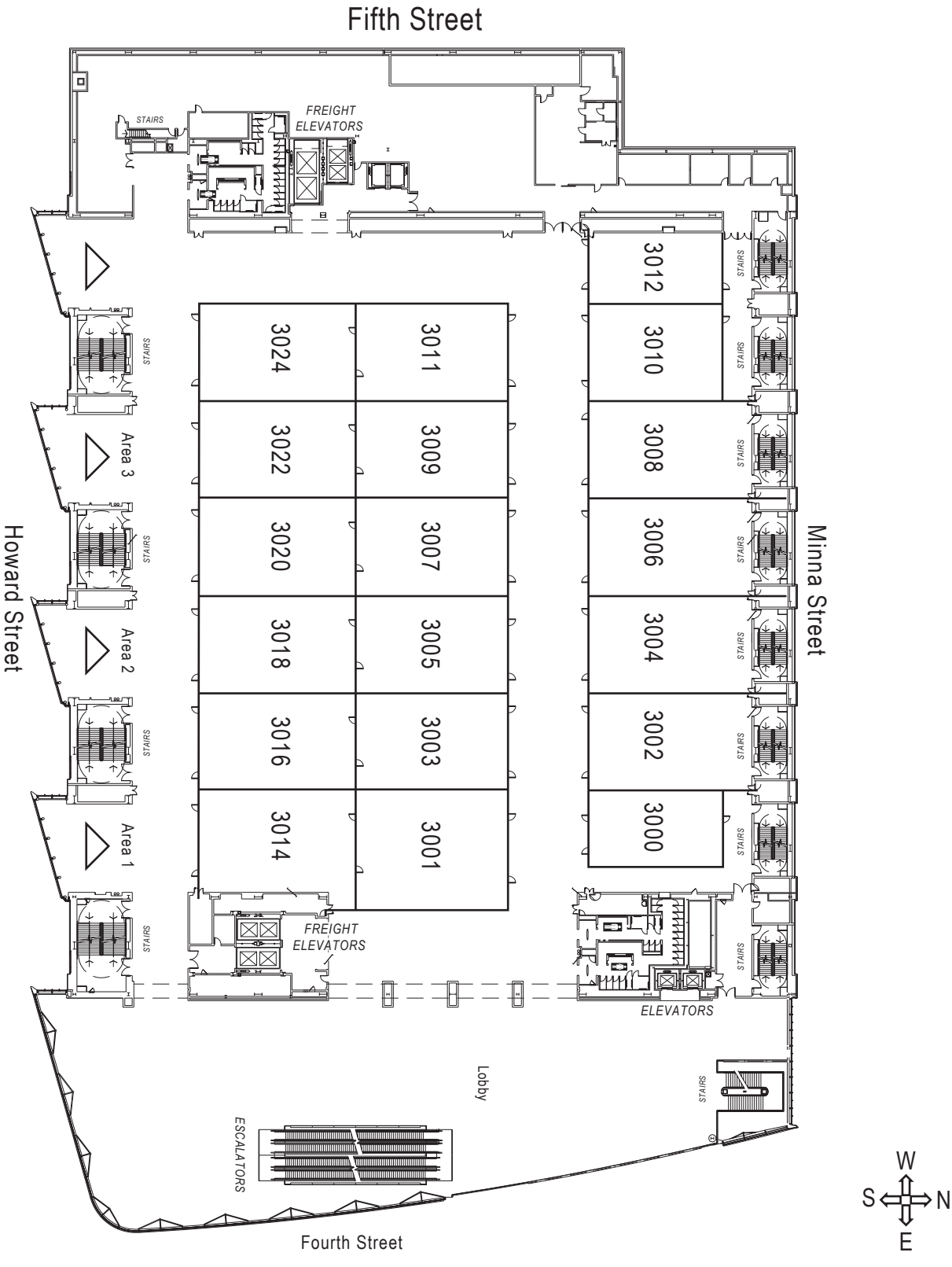
MOSCONE WEST

Level 2



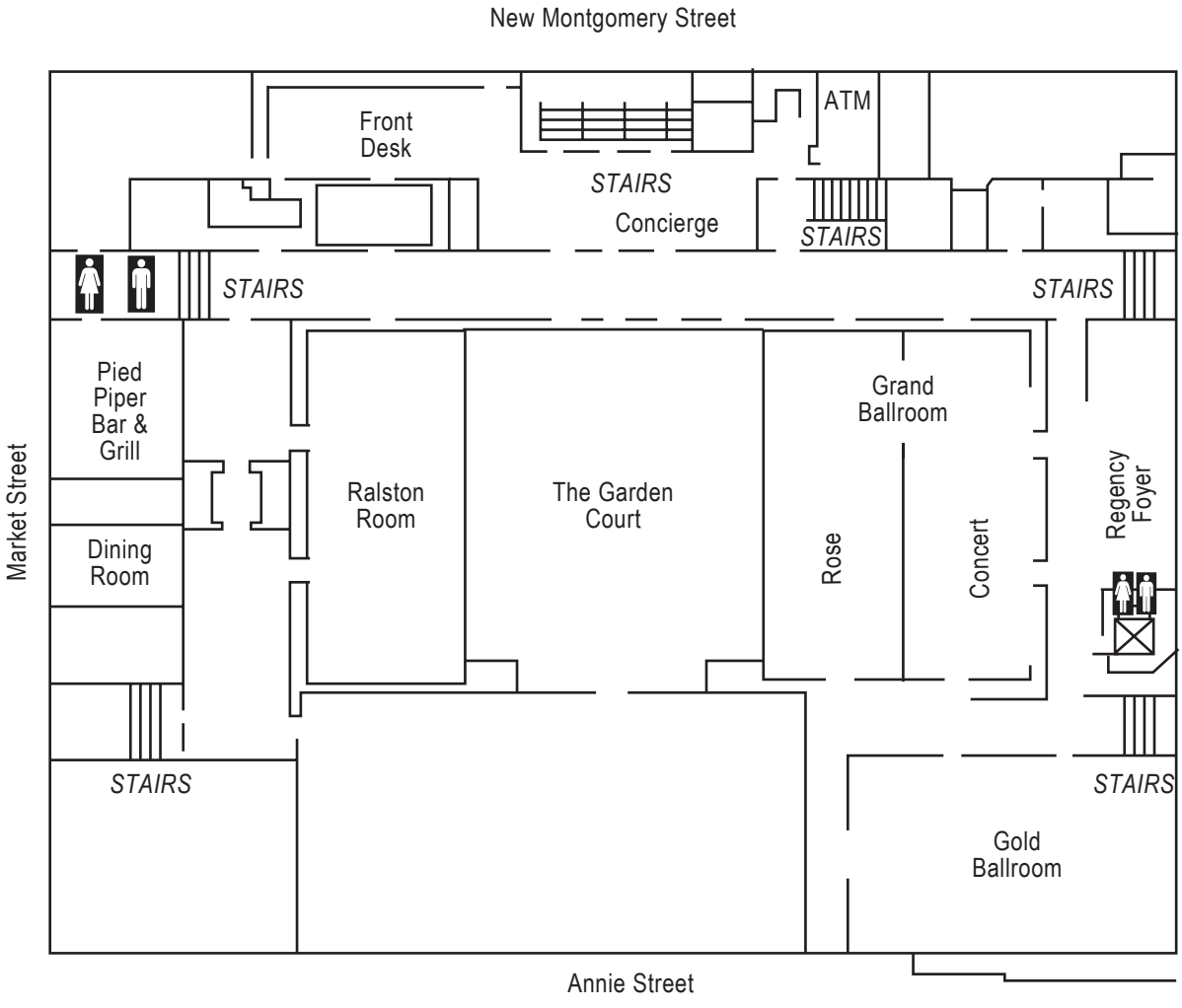
MOSCONE WEST

Level 3

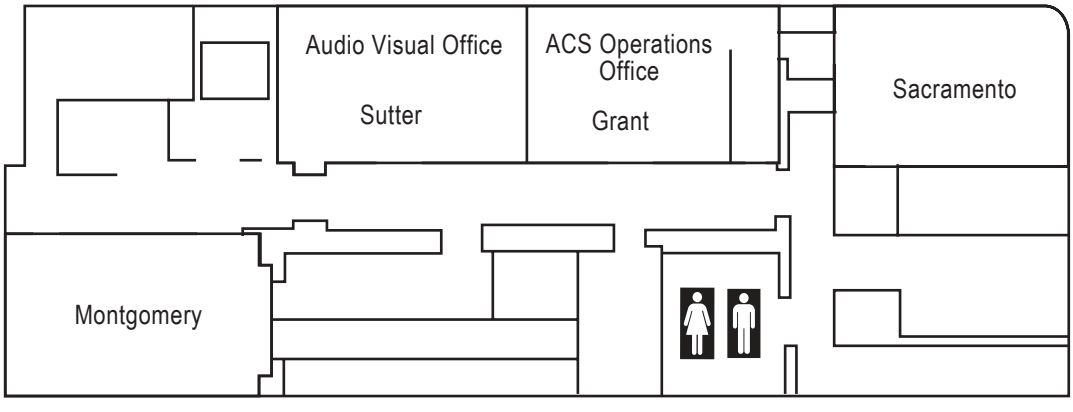


PALACE HOTEL

Lobby Level

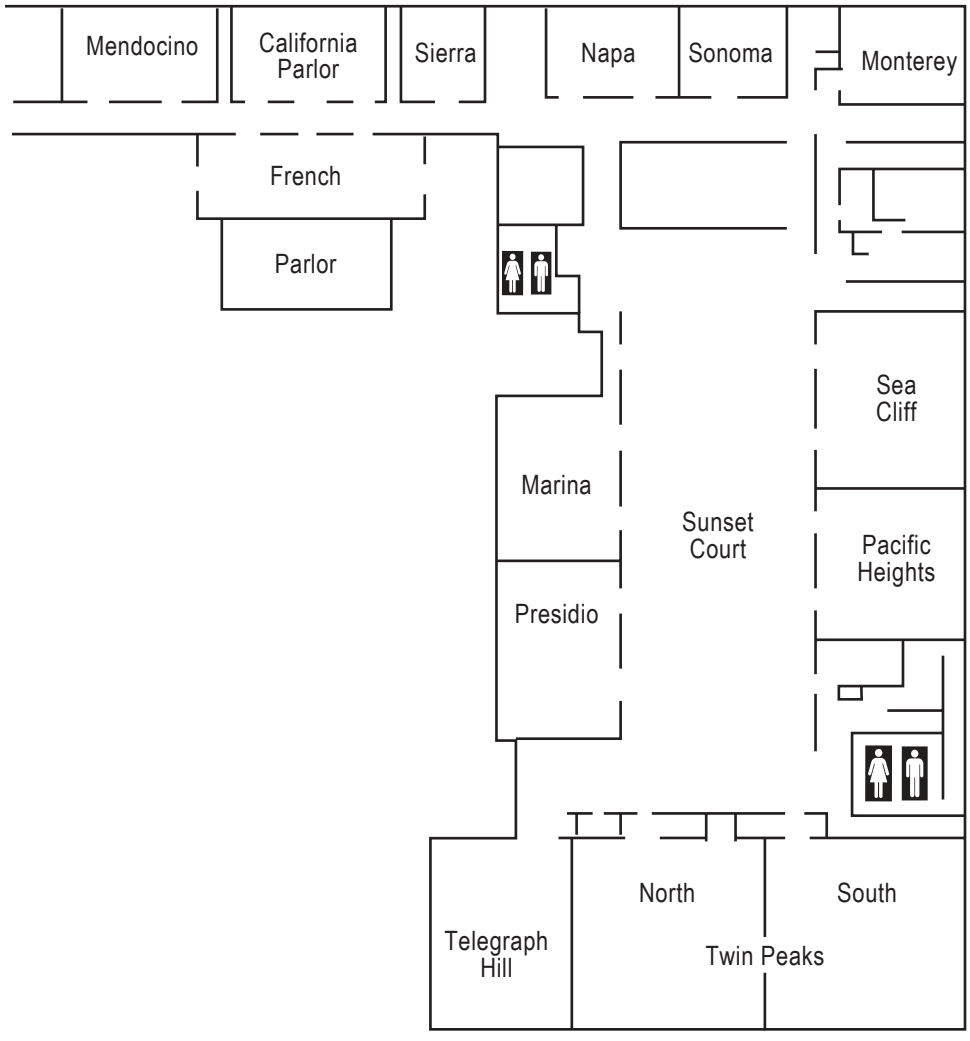


Mezzanine



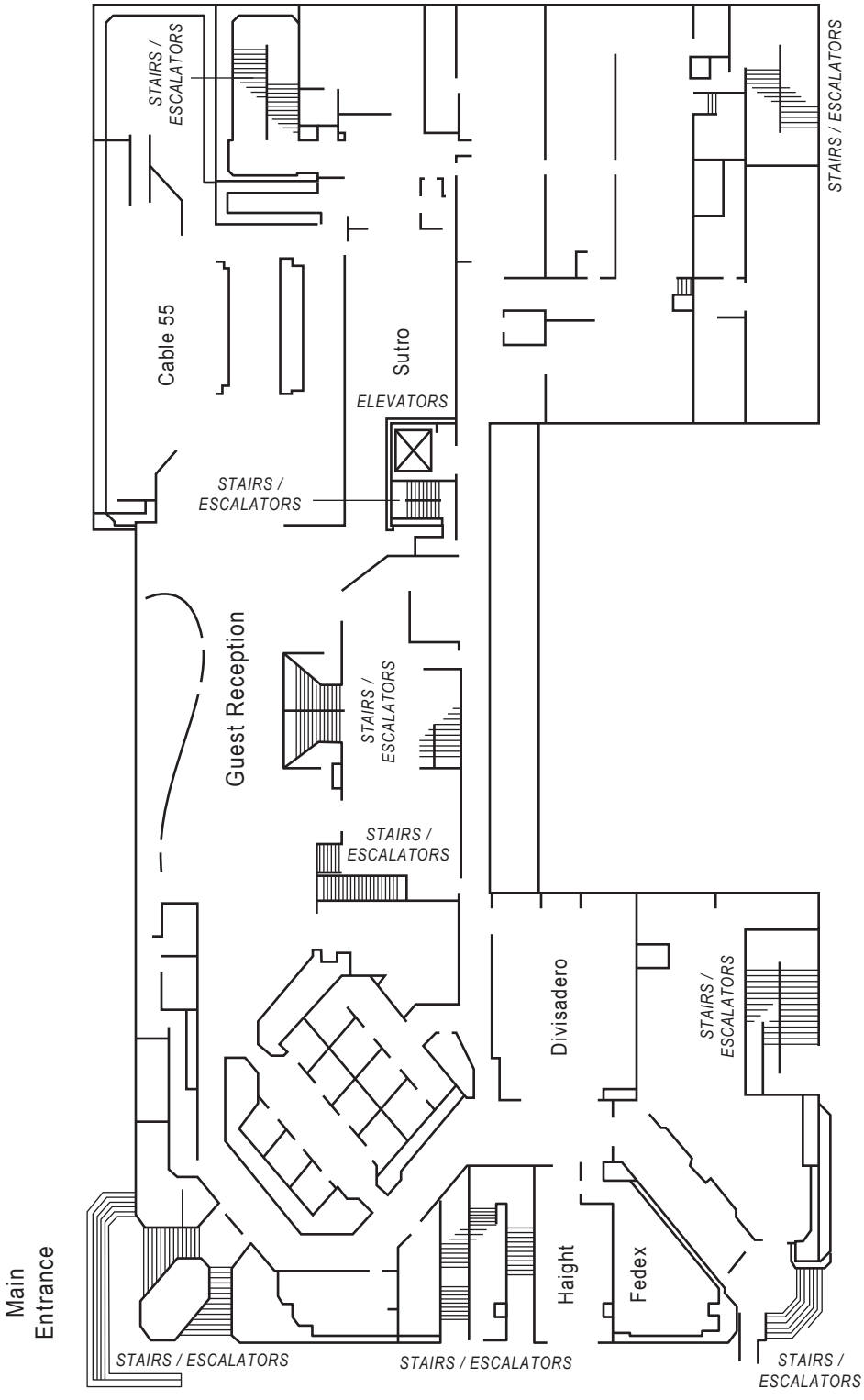
PALACE HOTEL

Second Level



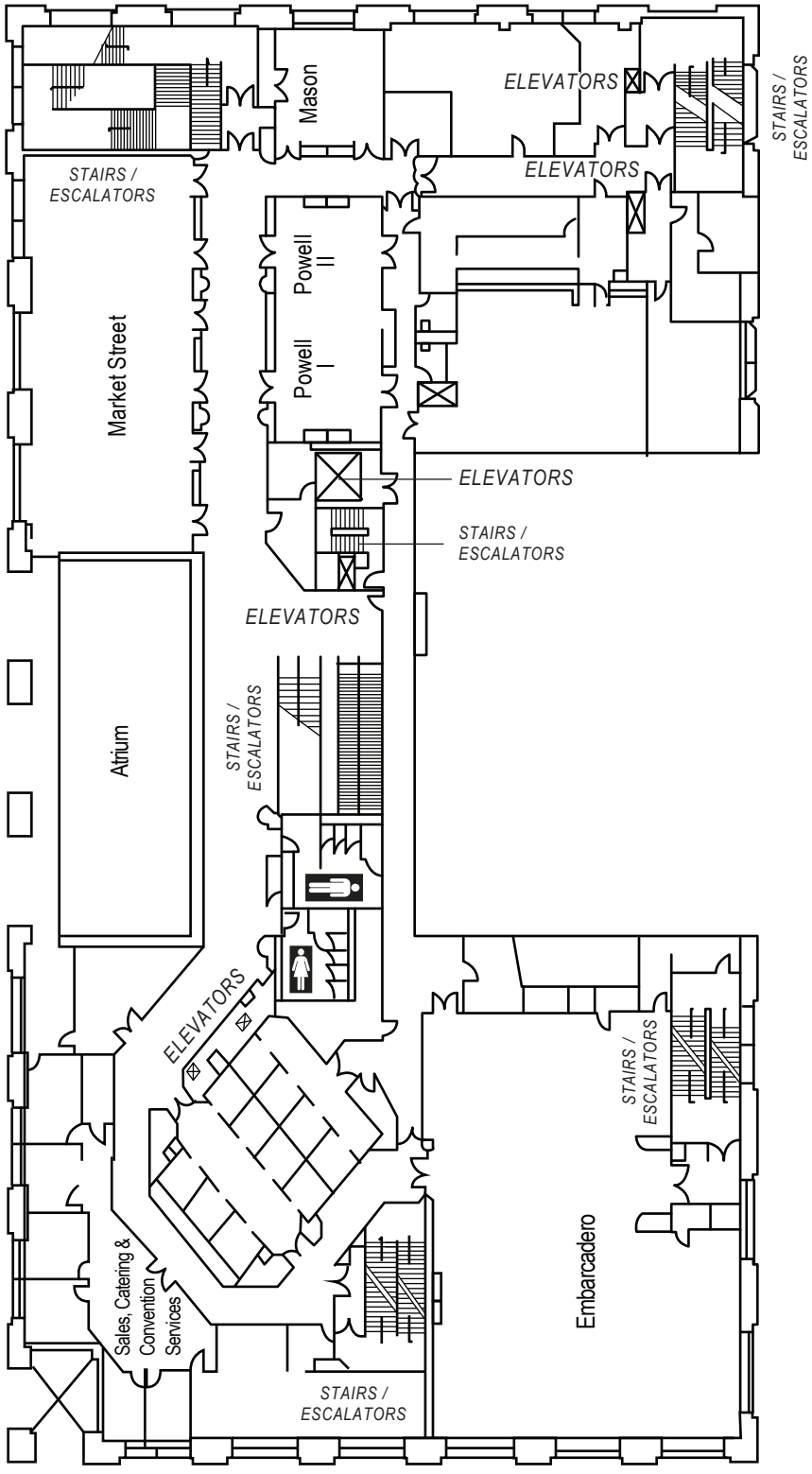
PARC 55

Level two



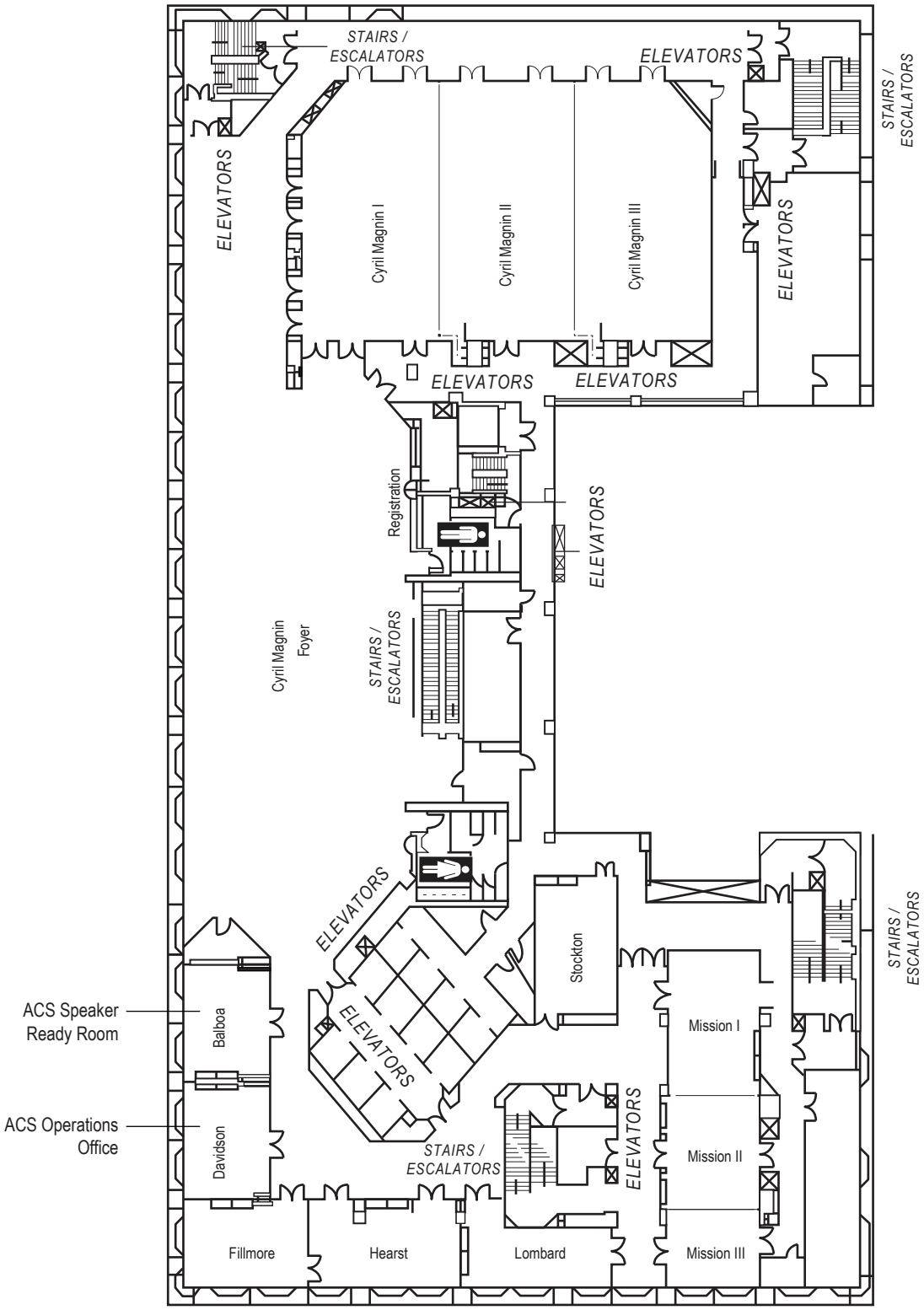
PARC 55

3rd Floor



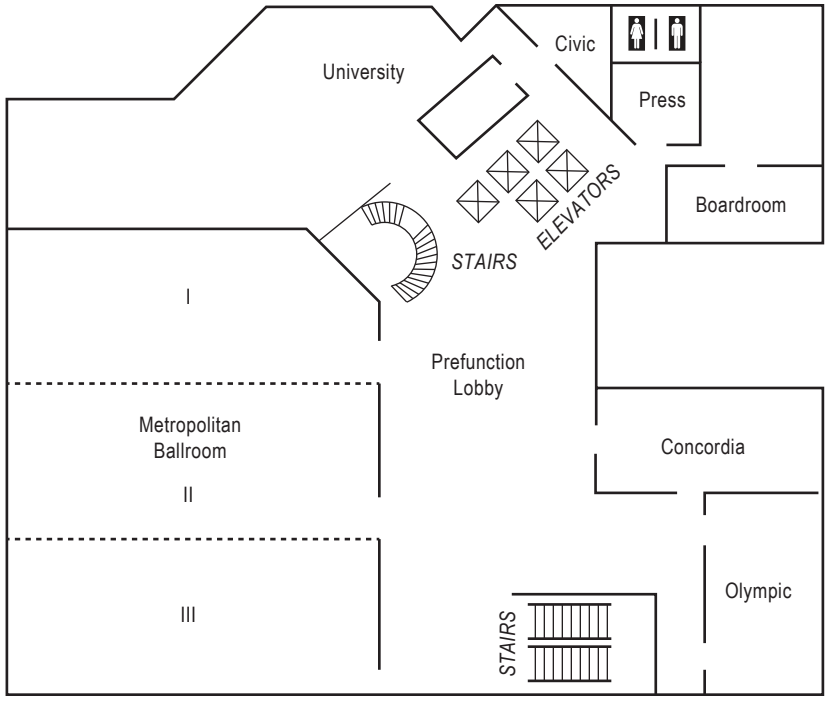
PARC 55

4th Floor

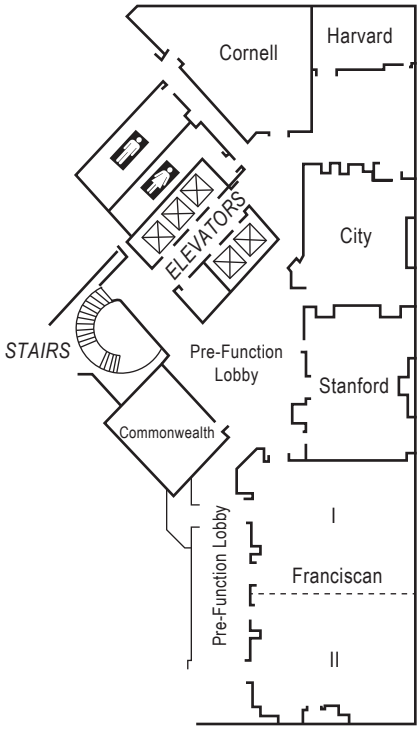


PARK CENTRAL

Second Floor

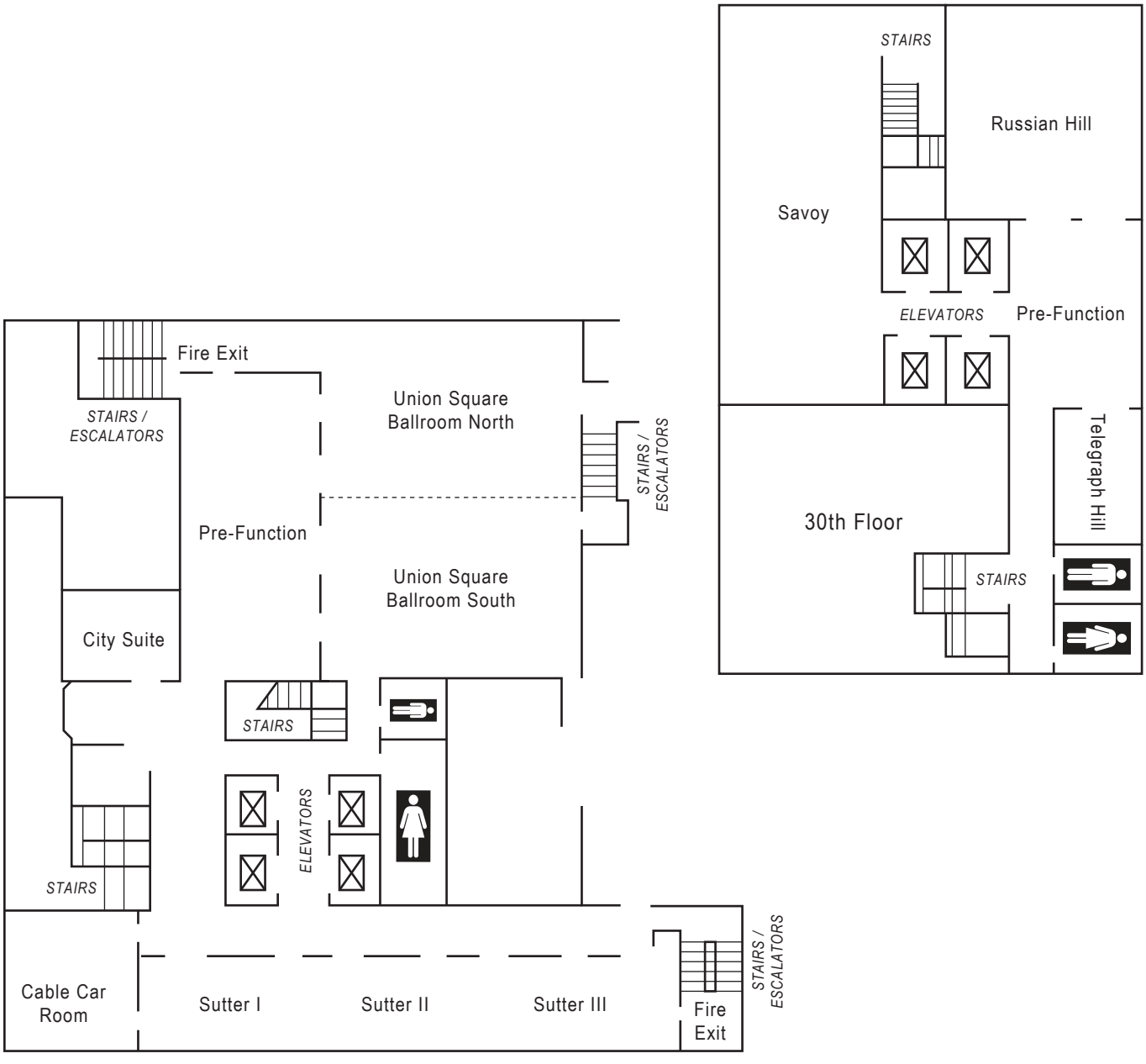


Third Floor



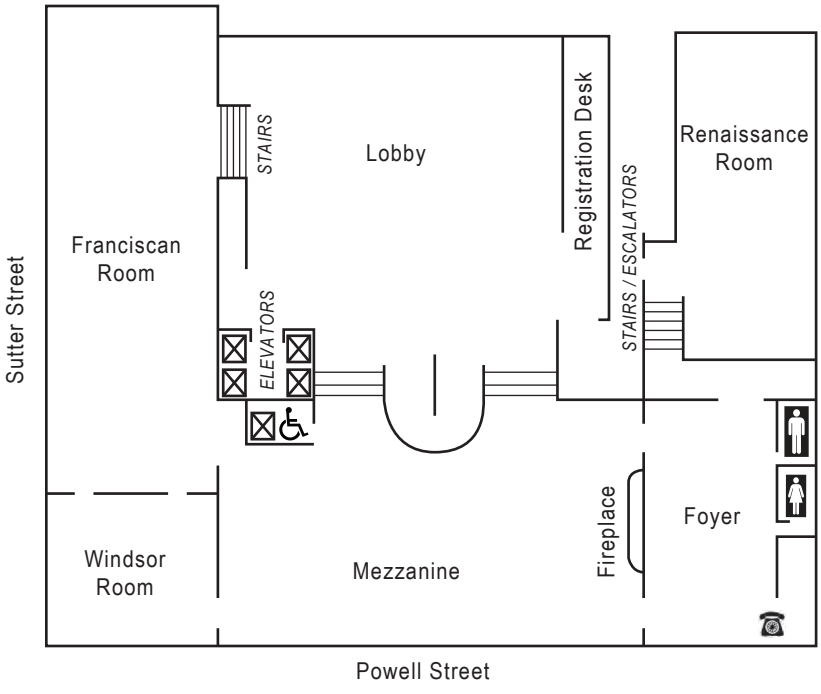
SAN FRANCISCO MARRIOTT UNION SQUARE

Mezzanine Level

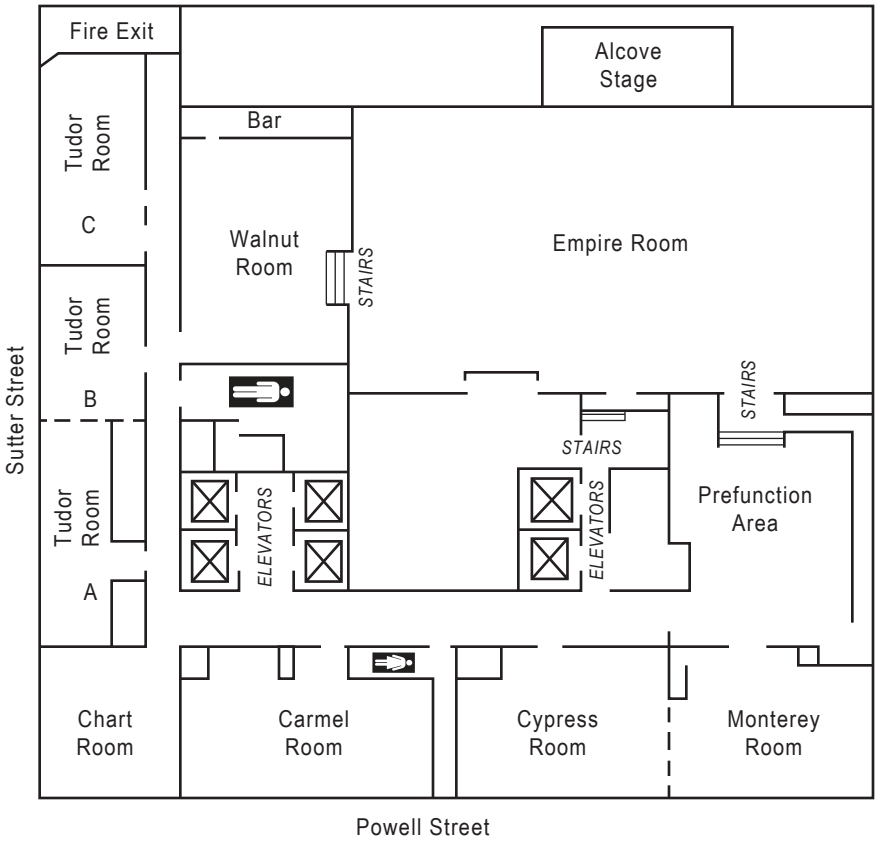


SAN FRANCISCO MARRIOTT UNION SQUARE

Mezzanine Level

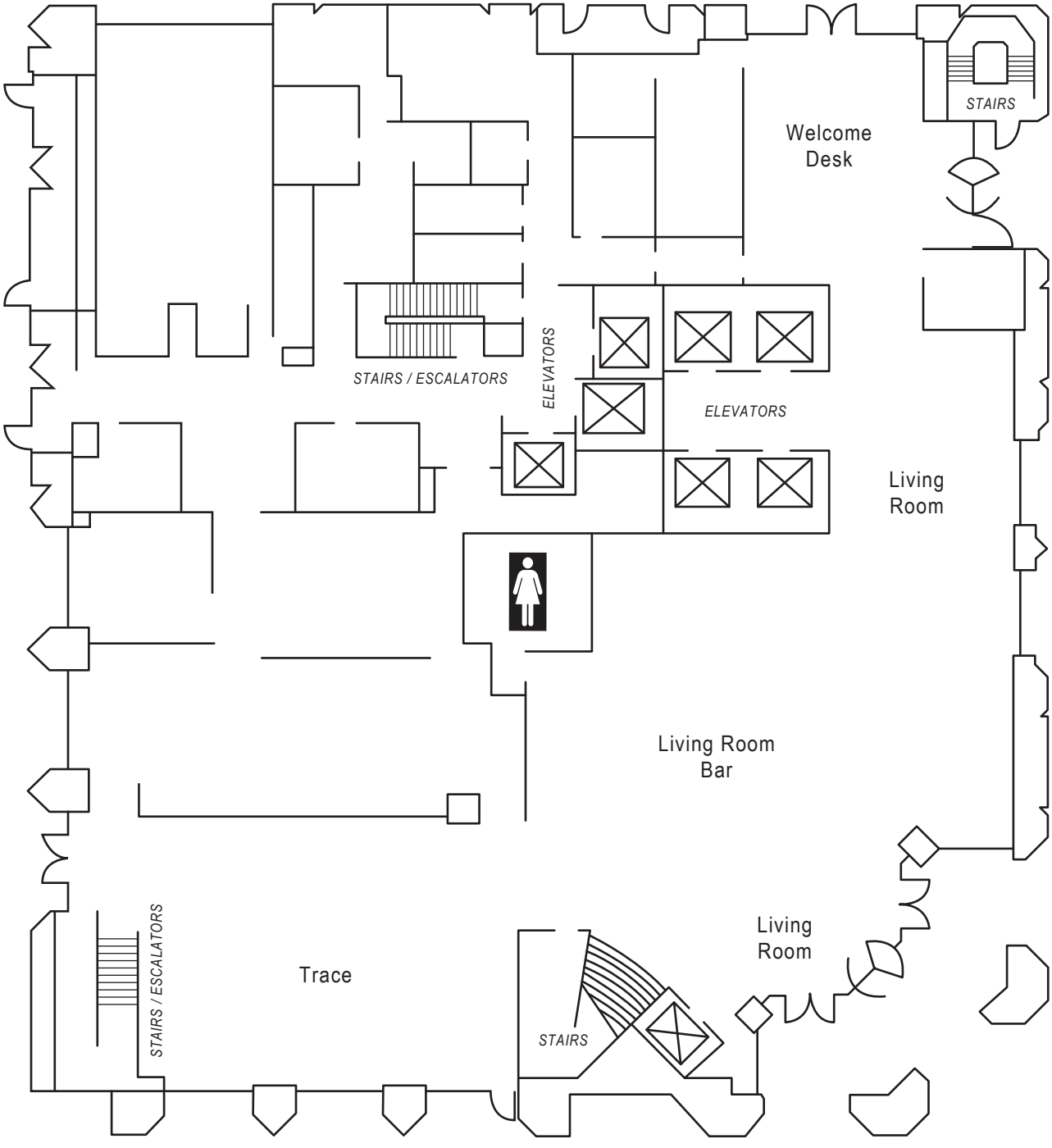


Second Floor



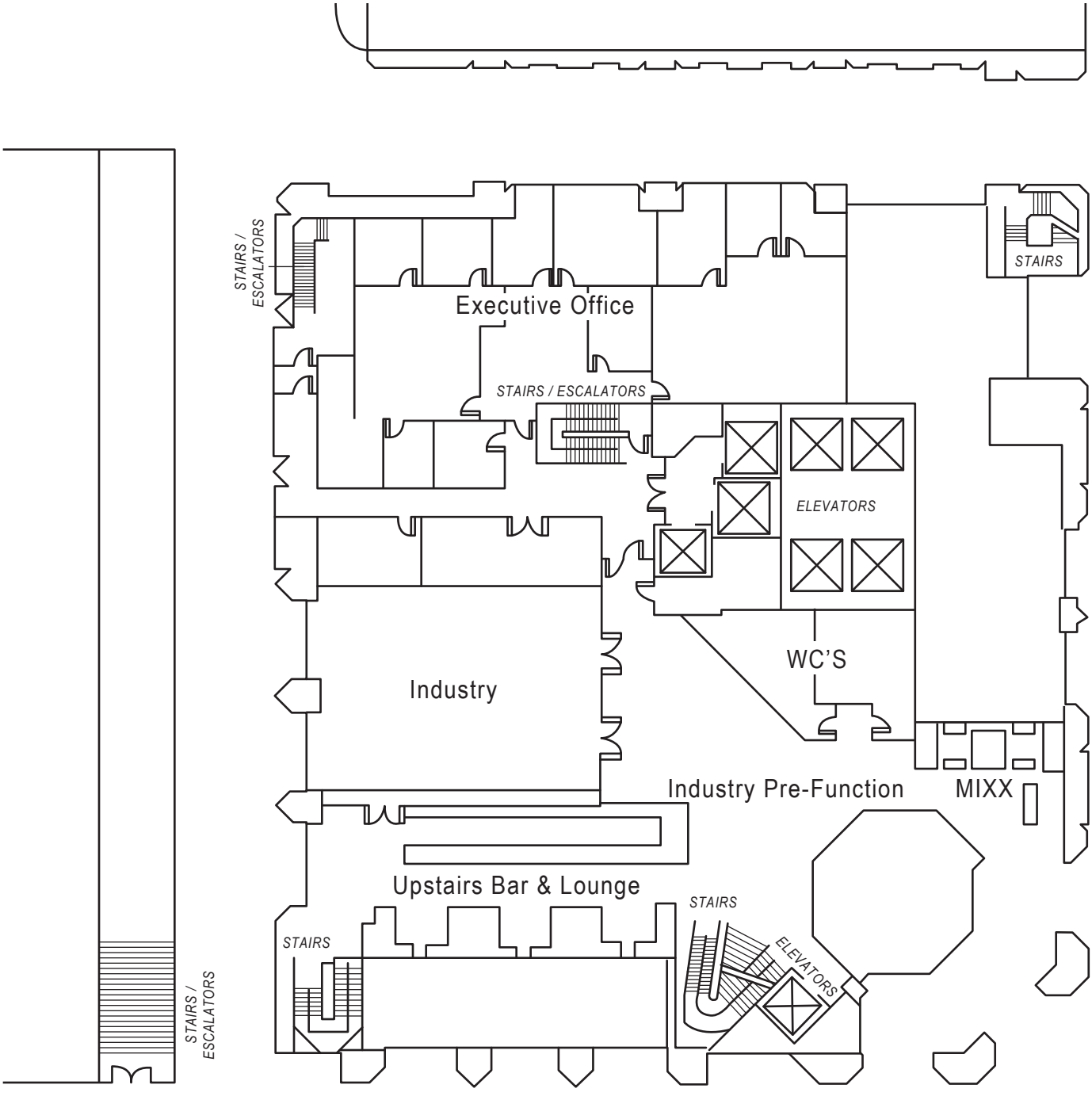
WESTIN ST. FRANCIS

First Floor



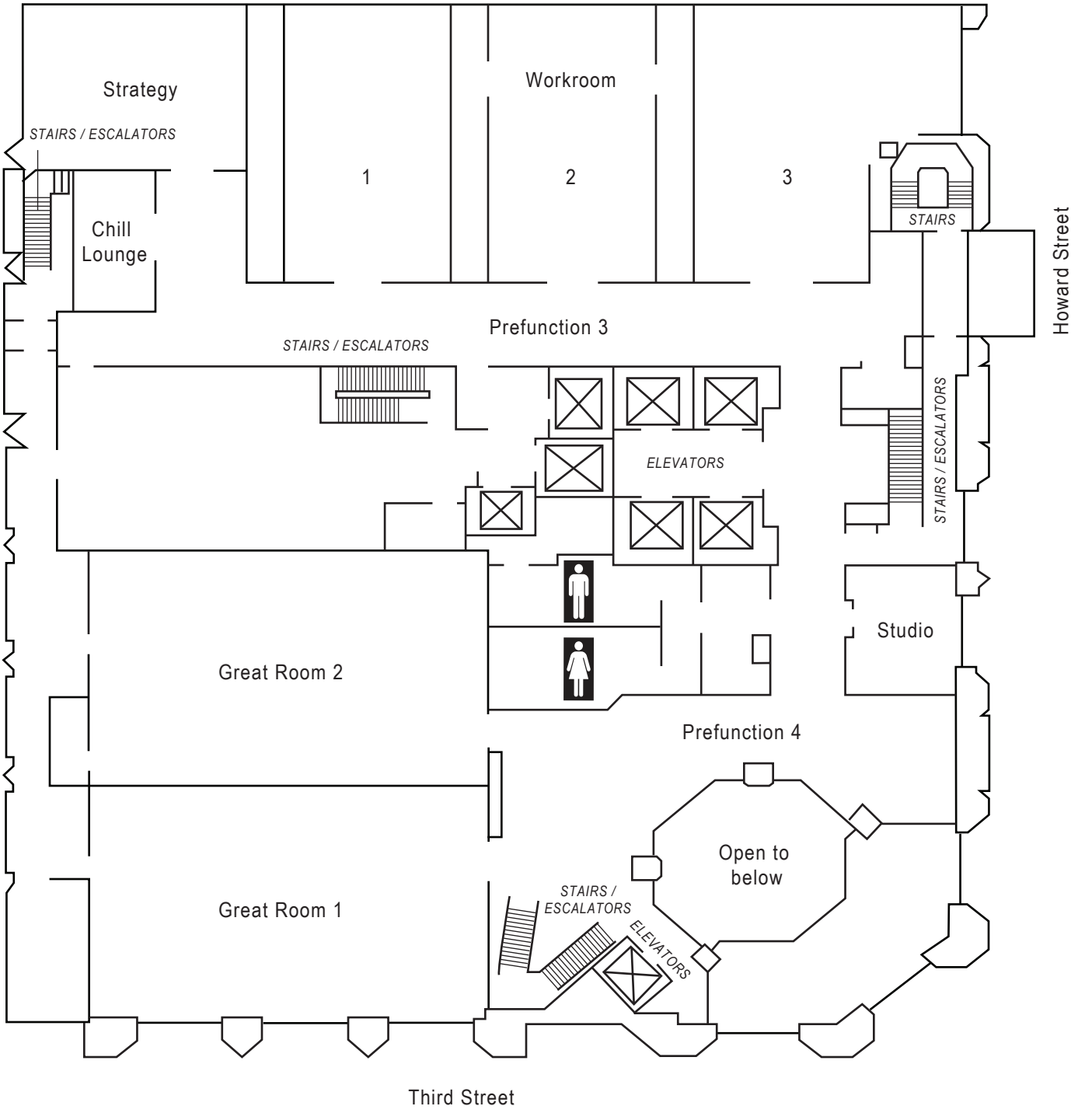
WESTIN ST. FRANCIS

Second Floor



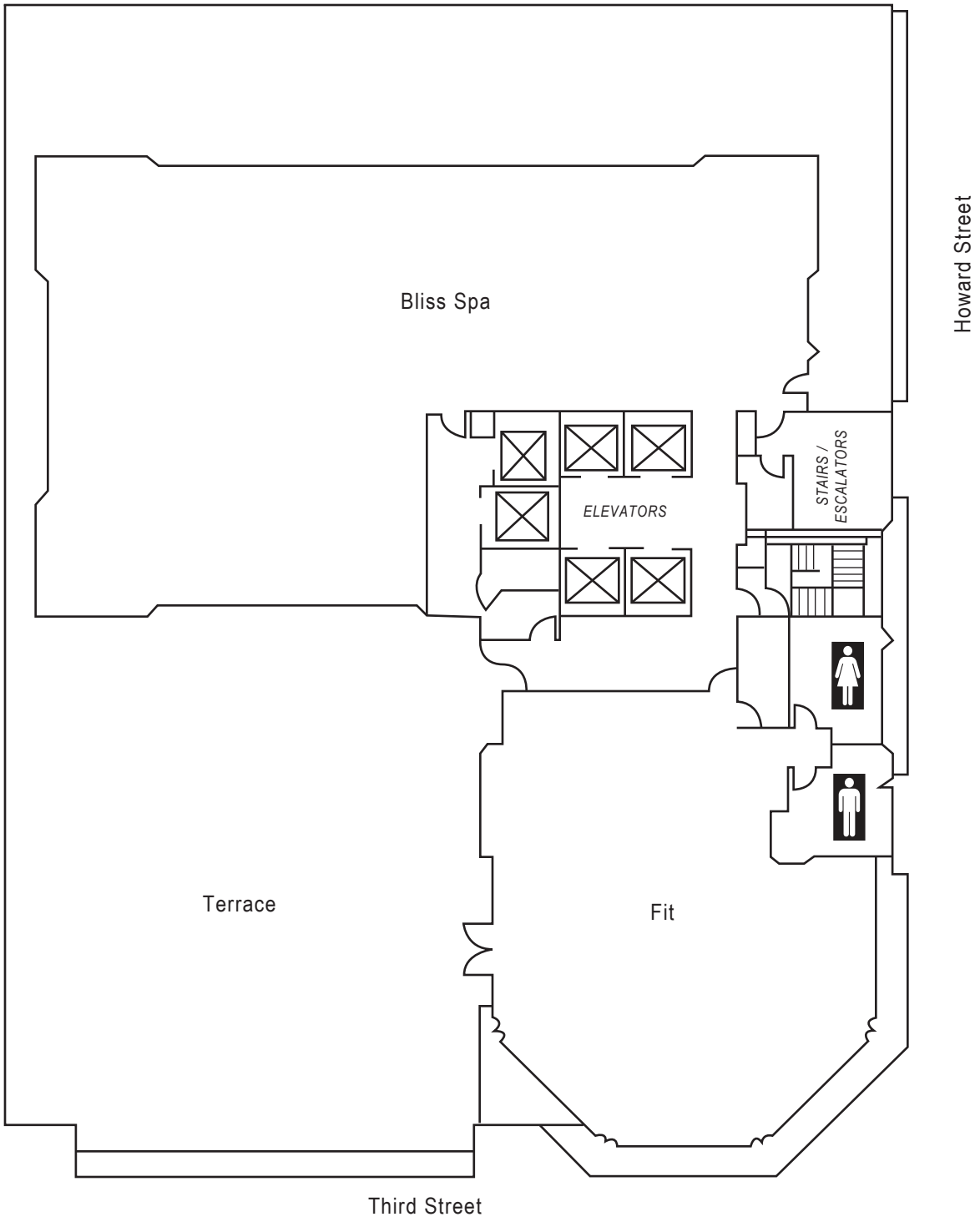
WESTIN SAN FRANCISCO

Third Floor Function Space



WESTIN SAN FRANCISCO

Fourth Floor Function Space



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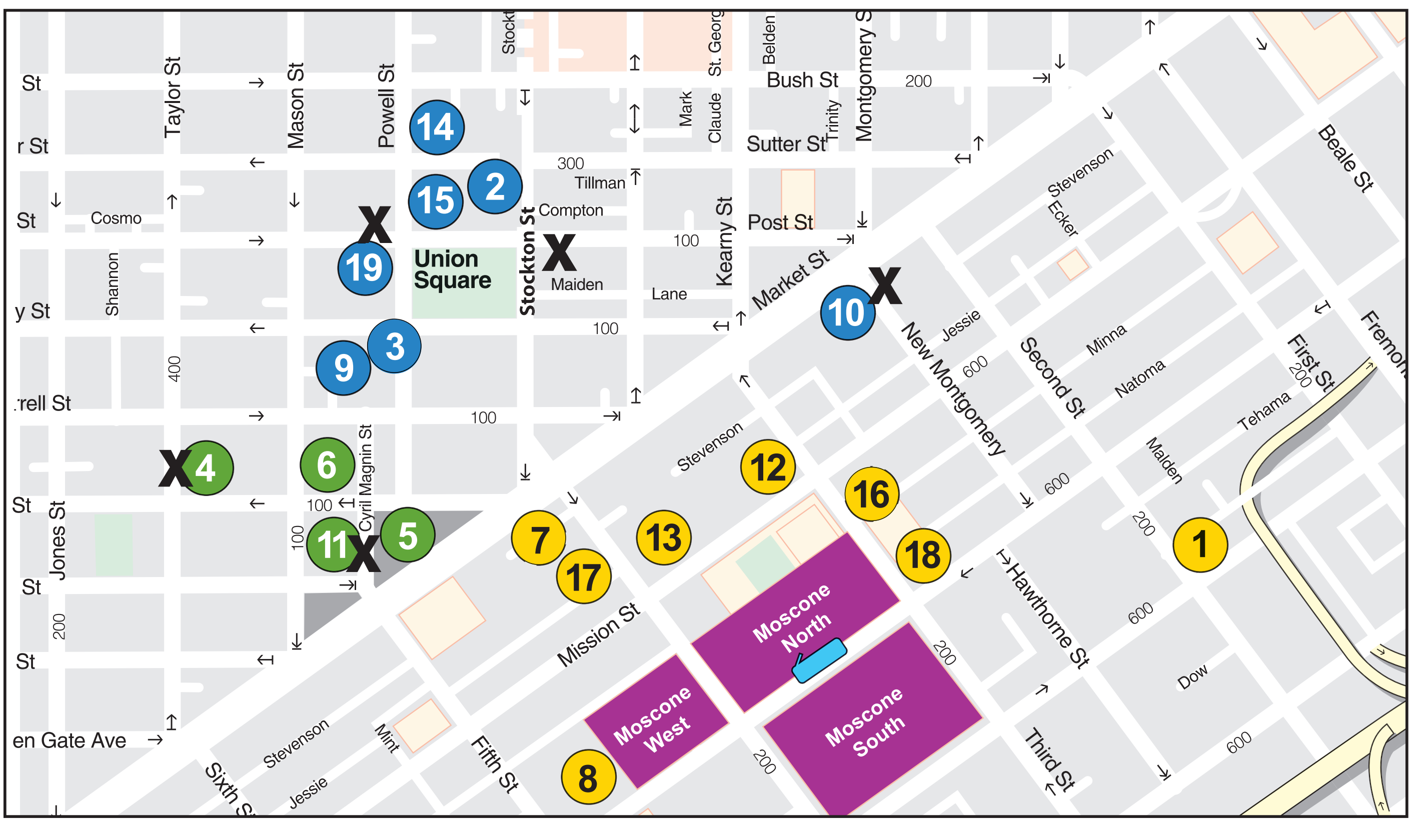


Shuttle information

Shuttle Schedule

SUNDAY, APRIL 2*

7:00 AM – 10:00 AM ..... 15 minute service
10:00 AM – 4:00 PM ..... 30 minute service
4:00 PM – 7:00 PM ..... 15 minute service
7:00 PM – 11:00 PM ..... 30 minute service

MONDAY, APRIL 3

7:00 AM – 10:00 AM ..... 15 minute service
10:00 AM – 4:00 PM ..... 30 minute service
4:00 PM – 11:00 PM ..... 15 minute service

TUESDAY, APRIL 4

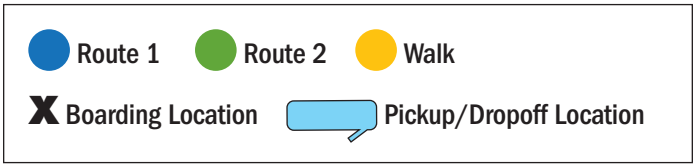
7:00 AM – 10:00 AM ..... 15 minute service
10:00 AM – 4:00 PM ..... 30 minute service
4:00 PM – 11:00 PM ..... 15 minute service

WEDNESDAY, APRIL 5

6:30 AM – 11:00 PM ..... 30 minute service

THURSDAY, APRIL 6

7:00 AM – 6:00 PM..... 60 minute service



For all shutte enquiries and wheelchair assistance, please call 1-866-439-8564.

Shuttle Services managed and operated by Transportation Management Services.

Carbon Neutral Shuttles.

Scan here to download a copy of the shuttle schedule:

Visit our website at **www.acs.org/sanfran2017** to view a list of economical hotels.

American Chemical Society

Volunteer/National Meeting Attendee Conduct Policy

One of the key strengths of the ACS has been the enduring and varied contributions made by its thousands of dedicated volunteers.

Another unassailable strength of the ACS is its outstanding national meetings program. ACS national meetings are among the most respected scientific meetings in the world. ACS national meetings offer scientific professionals a legitimate platform to present, publish, discuss, and exhibit the most exciting research discoveries and technologies in chemistry and its related disciplines. Furthermore, ACS national meetings facilitate networking opportunities, career development and placement, and provide organizations with opportunities to exhibit products and services to targeted audiences.

The Society's Congressional Charter explicitly lists among its objectives "the improvement of the qualifications and usefulness of chemists through high standards of professional ethics, education and attainments...." The ACS expects its volunteers and national meeting attendees to display the highest qualities of personal and professional integrity in all aspects of their ACS-related activities. Indeed, every chemical professional has obligations to the public, to volunteer and staff colleagues, and to science.

Accordingly, and to foster a positive environment built upon a foundation of trust, respect, open communications, and ethical behavior, the ACS Board of Directors has issued this Conduct Policy. It applies to ACS Volunteers, i.e., it applies to individuals conducting the business and affairs of the ACS without compensation for that conduct. It also applies to attendees at ACS national meetings. Volunteers and national meeting attendees should at all times abide by this Conduct Policy. Specifically:

1. Volunteers should understand and support ACS's vision and mission.

2. Volunteers and national meeting attendees should contribute to a collegial, inclusive, positive, and respectful environment for their fellow volunteers and attendees, as well as for other stakeholders, including national meeting vendors and ACS staff.

3. Volunteers and national meeting attendees must avoid taking any inappropriate actions based on race, gen- der, age, religion, ethnicity, nationality, sexual orientation, gender expression, gender identity, marital status, political affiliation, presence of disabilities, or educational background. They should show consistent respect to colleagues, regardless of the level of their formal education and whether they are from industry, government or academia, or other scientific and engineering disciplines.

4. Volunteers and national meeting attendees should interact with others in a cooperative and respectful manner. Volunteers and national meeting attendees should refrain from using insulting, harassing, or otherwise offensive language in their ACS interactions. Disruptive, harassing, or inappropriate behavior toward other volunteers, stakeholders, or staff is unacceptable. Personal boundaries set by others must be observed. Harassment of any kind, including but not limited to unwelcome sexual advances, requests for sexual favors, and other verbal or physical harassment will not be tolerated.

5. Volunteers must obey all applicable laws and regulations of the relevant government authorities while acting on behalf of the ACS. Likewise, national meeting attendees must obey all applicable laws and regulations of the relevant government authorities while attending ACS national meetings. Volunteers and national meeting attendees alike should also ensure that they comply with all applicable safety guidelines relating to public chemistry demonstrations.

6. Volunteers and national meeting attendees should only use ACS's trademarks, insignia, name, logos, and other intellectual property in compliance with ACS regulations and directives as may be issued from time to time.

7. Violations of this Conduct Policy should be reported promptly to the ACS Secretary and General Counsel or to the Chair of the ACS Board of Directors. In cases of alleged persistent and/or serious violations of this Conduct Policy, the Board shall review the evidence and shall take such actions as may be appropriate, including but not limited to requiring volunteers to leave their volunteer position(s); precluding volunteers from serving in Society volunteer roles in the future; requiring national meeting attendees to leave the meeting; and, precluding meeting attendees from attending future ACS national meetings. ACS, through its Board of Directors, reserves the right to pursue additional measures as it may determine are appropriate.

Adopted by the Board of Directors 12/6/13