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9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS (ES) U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211			10. SPONSOR/MONITOR'S ACRONYM(S) ARO		
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a. REPORT	b. ABSTRACT	c. THIS PAGE			Gilbert Nathanson
UU	UU	UU	UU		19b. TELEPHONE NUMBER 608-262-8098

RPPR Final Report
as of 21-Sep-2018

Agency Code:

Proposal Number: 69098CHCF

Agreement Number: W911NF-16-1-0137

INVESTIGATOR(S):

Name: Gilbert Nathanson
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Organization: **Gordon Research Conferences, Inc.**

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DUNS Number: 075712877

EIN: 050300482

Report Date: 14-Jan-2017

Date Received: 21-Aug-2018

Final Report for Period Beginning 15-Apr-2016 and Ending 14-Oct-2016

Title: 2016 Molecular Interactions and Dynamics Gordon Research Conference and Gordon Research Seminar

Begin Performance Period: 15-Apr-2016

End Performance Period: 14-Oct-2016

Report Term: 0-Other

Submitted By: Nancy Ryan Gray

Email: grants@grc.org

Phone: (401) 360-1505

Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees:

STEM Participants:

Major Goals: Organizing a Gordon Research Conference involves extensive communication with the research community to identify important issues at the frontiers of the field, and solicit suggestions for speakers and discussion leaders to participate in the conference. The Chair then contacts prospective participants to invite them to talk and discuss the nature of their contributions. The Chair then communicates the topics and aims of the conference through web pages, contact with relevant international professional bodies and email to members of the research community around the world to encourage applications for participation in the conference. The Chair is then responsible for assessing and accepting the applications and fielding a host of questions both concerning the technical content and practical aspects of conference participation.

Accomplishments: The new Molecular Interactions and Dynamics Gordon Conference merged two GRCs with long and distinguished histories: the Atomic and Molecular Interactions GRC and the Molecular Energy Transfer GRC. These meetings have traditionally involved scientists engaged in fundamental research at the molecular level in gas and condensed phases and at surfaces and those who apply these concepts to systems of practical chemical and physical interest. A key tradition in these meetings is the strong mix of theory and experiment and the dialogue it stimulates. The 2016 MID conference proudly continued these traditions. The conference hosted talks in the diverse areas of:

- ? Reactions in the Atmosphere: Energy and Climate
- ? Intermolecular Interactions and Dynamics
- ? Dynamics of Biological Systems
- ? Interactions and Dynamics in Materials
- ? Dynamics and Reactions in Solutions and in Clusters
- ? Interfacial Dynamics and Reactions
- ? Unraveling the Dynamics of Catalytic Reactions
- ? Photochemistry and Nonadiabatic Dynamics
- ? New Horizons in Intermolecular Interactions

These topics span a wide range of disciplines, grounded in physical chemistry, and reaching into atmospheric chemistry, biology, catalysis, materials, and energy-related science. The Conference brought together investigators who are at the forefront of these fields, and provided opportunities for junior scientists and graduate students to present their work in poster format and exchange ideas with established leaders. Several poster presenters were selected for short talks based on the abstracts provided. The collegial atmosphere of this Conference provided an avenue for scientists of all ages and disciplines to get to know each other, to brainstorm new ideas, and to establish

RPPR Final Report as of 21-Sep-2018

fruitful collaborations.

In keeping with the traditions of both the Atomic and Molecular Interactions and the Molecular Energy Transfer Gordon Research Conferences, the Gordon Research Seminar on Molecular Interactions and Dynamics encompassed areas of fundamental research in chemical physics, focusing on gas and condensed phases, interfaces, and the application of fundamental ideas to practical chemical fields. There was a strong mix of theoretical and experimental research, facilitating networking and future collaborations.

Training Opportunities: Speakers, discussion leaders, poster presenters and attendees simultaneously contributed to and benefited from the collective skills and experience shared throughout the conference.

Results Dissemination: The final program has been posted on the GRC website.

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report



GORDON RESEARCH CONFERENCES

FINAL PROGRESS REPORT

Army Research Office

Molecular Interactions & Dynamics GRC/GRS

Grant Number W911NF-16-1-0137

July 9-15, 2016

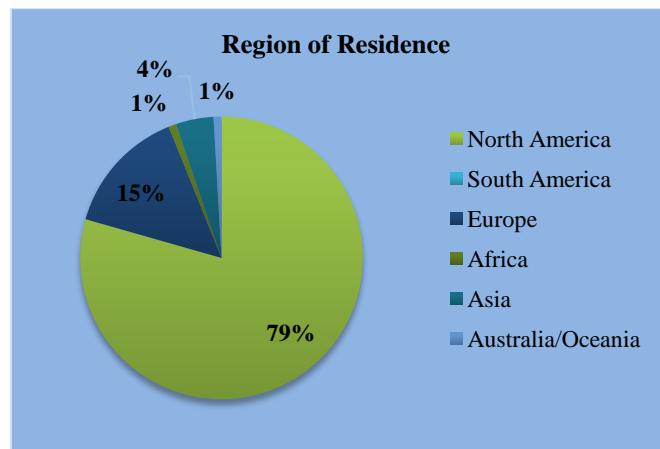
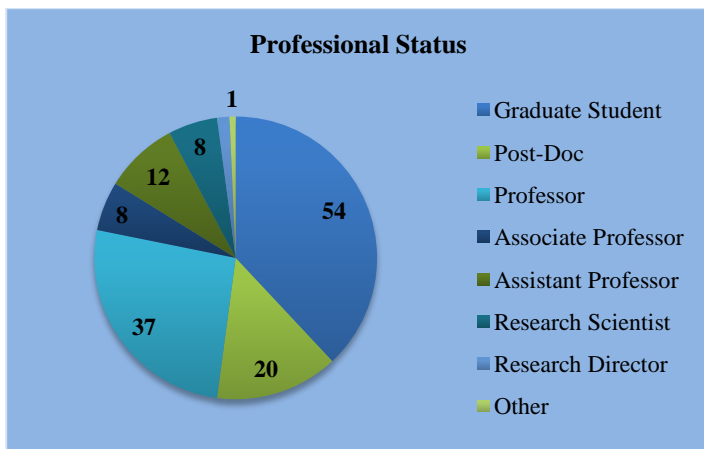
Operational Summary

The Gordon Research Conference (GRC) and Gordon Research Seminar (GRS) on Molecular Interactions & Dynamics were held at Stonehill College in Easton, Massachusetts from July 9-15, 2016. The meeting covered a variety of scientific topics and the content presented was highly rated by participants.



Conference Participants

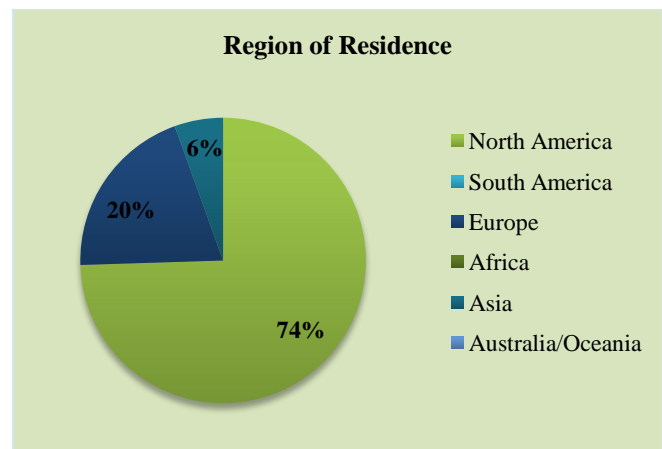
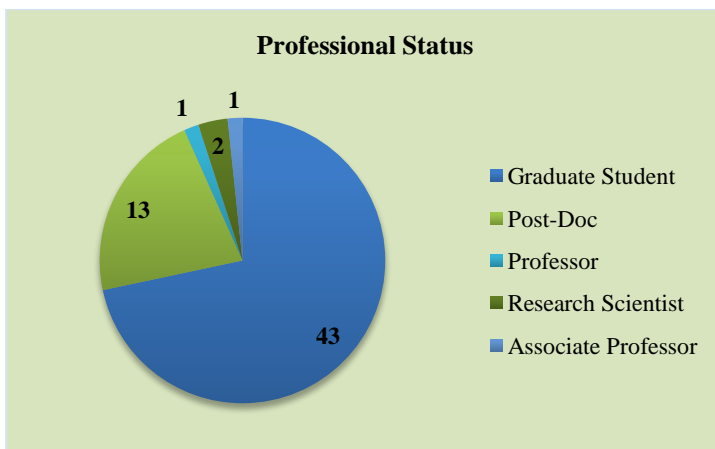
The Conference was well-attended with 142 participants. Scientists from academia represented 93% of the participants while attendees from government accounted for 7%. The meeting also attracted a strong mix of young investigators and senior scientists. Students and post-docs accounted for 52% of all attendees. Approximately 32% of the participants at the 2016 meeting were women.



Gordon Research Seminars

Seminar Participants

The Seminar was well-attended with 60 participants. Scientists from academia represented 95% of the participants while attendees from government accounted for 3% and 2% from industry. Students and post docs combined accounted for 94% of all attendees. Approximately 37% of the participants at the 2016 seminar were women.



Conference Program

The new Molecular Interactions and Dynamics Gordon Conference merged two GRCs with long and distinguished histories: the Atomic and Molecular Interactions GRC and the Molecular Energy Transfer GRC. These meetings have traditionally involved scientists engaged in fundamental research at the molecular level in gas and condensed phases and at surfaces and those who apply these concepts to systems of practical chemical and physical interest. A key tradition in these meetings is the strong mix of theory and experiment and the dialogue it stimulates. The 2016 MID conference proudly continued these traditions. The conference hosted talks in the diverse areas of:

- Reactions in the Atmosphere: Energy and Climate
- Intermolecular Interactions and Dynamics
- Dynamics of Biological Systems
- Interactions and Dynamics in Materials
- Dynamics and Reactions in Solutions and in Clusters
- Interfacial Dynamics and Reactions
- Unraveling the Dynamics of Catalytic Reactions
- Photochemistry and Nonadiabatic Dynamics
- New Horizons in Intermolecular Interactions

These topics span a wide range of disciplines, grounded in physical chemistry, and reaching into atmospheric chemistry, biology, catalysis, materials, and energy-related science. The Conference brought together investigators who are at the forefront of these fields, and provided opportunities for junior scientists and graduate students to present their work in poster format and exchange ideas with established leaders. Several poster presenters were selected for short talks based on the abstracts provided. The collegial atmosphere of this Conference provided an avenue for scientists of all ages and disciplines to get to know each other, to brainstorm new ideas, and to establish fruitful collaborations.

In keeping with the traditions of both the Atomic and Molecular Interactions and the Molecular Energy Transfer Gordon Research Conferences, the Gordon Research Seminar on Molecular Interactions and Dynamics encompassed areas of fundamental research in chemical physics, focusing on gas and condensed phases, interfaces, and the application of fundamental ideas to practical chemical fields. There was a strong mix of theoretical and experimental research, facilitating networking and future collaborations.

Conference Budget

Funding provided by the Army Research Office supported partial registration for 6 postdocs and 13 graduate students at the GRC and partial registration for 5 postdocs and 13 graduate students at the GRS.

Conference Feedback

Participants had an opportunity to provide feedback at the end of the Conference. The feedback collected from the meeting was extremely positive. Evaluations included numerous positive remarks regarding the power hour, networking opportunities and the diversity of the topics and speakers. Evaluations from the GRS included positive comments regarding the conversations about techniques with others using similar instruments, the opportunity to have an active role in the seminar and the career panel.

GRC would like to thank the Army Research Office for its continued support of the meetings. The contributions received from the Army Research Office have been critical to the success of the conferences and are having a measurable impact in advancing the frontiers of science worldwide.

Dr. Gilbert Nathanson, GRC Chair
University of Wisconsin-Madison

Dr. Olga Gorlova, GRS Chair
Yale University

Dr. Nancy Ryan Gray
President and Chief Executive Officer
Gordon Research Conferences

Molecular Interactions & Dynamics

Gordon Research Conference

Energy Transfer and Dynamics of Chemical Reactions Involving Isolated Molecules, Clusters, Interfaces, Solutions, Materials,
and Biological Systems

July 10-15, 2016

Stonehill College

Easton, MA

Chairs: [Gilbert M. Nathanson](#) & [Spiridoula Matsika](#)

Vice Chair: [Richard A. Loomis](#)

Contributors



Meeting Program

Sunday

2:00 pm - 9:00 pm	Arrival and Check-in
6:00 pm	Dinner
7:30 pm - 7:35 pm	Welcome / Introductory Comments by GRC Site Staff
7:35 pm - 9:30 pm	Reactions in the Atmosphere: Energy and Climate Discussion Leader: Scott Kable (University of New South Wales, Australia)
7:35 pm - 8:05 pm	Marsha Lester (University of Pennsylvania, USA) "Dynamics of Hydrogen Transfer Reactions in Atmospheric Chemistry"
8:05 pm - 8:15 pm	Discussion
8:15 pm - 8:45 pm	Benny Gerber (University of California, Irvine, USA) "Mechanisms and Dynamics in Time of Acid Ionization on Liquid Water and Ice Surfaces"
8:45 pm - 8:55 pm	Discussion
8:55 pm - 9:25 pm	Nicholas Shuman (Air Force Research Laboratory, USA)

"Chemi-Ionization of Lanthanide Metals at 200 km"

9:25 pm - 9:30 pm Discussion

Monday

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Intermolecular Interactions and Dynamics**

Discussion Leader: **Timothy Zwier** (Purdue University, USA)

9:00 am - 9:30 am **Xueming Yang** (Dalian Institute of Chemical Physics, The Chinese Academy of Sciences, China)
"Dynamics of the O(1D) + CH₄ Reaction: Insertion or Abstraction"

9:30 am - 9:40 am Discussion

9:40 am - 10:10 am **Joel Bowman** (Emory University, USA)
"*Ab Initio* Potentials and Dynamics in High Dimensionality: Applications Ranging from the IR Spectroscopy of Methane Hydrate Clathrates to Energy Transfer in Gas-Phase Methane Collisions with Water"

10:10 am - 10:20 am Discussion

10:20 am - 10:50 am Coffee Break

10:50 am - 11:20 am **Sotiris Xantheas** (Pacific Northwest National Laboratory, USA)
"Stabilization and Reactivity of Multi-Valent Metal Cations in an Aqueous Environment: The Role of Excited States"

11:20 am - 11:30 am Discussion

11:30 am - 12:00 pm **Heather Lewandowski** (University of Colorado Boulder, USA)
"Chemical Reactions of Cold Molecular Ions and Molecular Radicals"

12:00 pm - 12:10 pm Discussion

12:10 pm - 12:25 pm **Wojciech Skomorowski** (University of Kassel, Germany)
"Quantum Phenomena in Low-Energy Penning Ionization Reaction with State-Selected Reactants"

12:25 pm - 12:30 pm Discussion

12:30 pm Lunch

1:30 pm - 4:00 pm Free Time

3:00 pm - 4:00 pm Power Hour

The GRC Power Hour is an optional informal gathering open to all meeting participants. It is designed to help address the challenges women face in science and support the professional growth of women in our communities by providing an open forum for discussion and mentoring.

Organizers: **Hanna Reisler** (University of Southern California, USA) and **Anne McCoy** (University of Washington, USA)

4:00 pm - 6:00 pm Poster Session

6:00 pm Dinner

7:30 pm - 9:30 pm **Dynamics of Biological Systems**

Discussion Leader: **Jan Verlet** (Durham University, United Kingdom)

7:30 pm - 8:00 pm **Christine Peter** (University of Konstanz, Germany)

"Challenges for the Development of Multiscale Simulation Models for Biomolecular Systems"

8:00 pm - 8:10 pm Discussion

8:10 pm - 8:40 pm **Christopher Cheatum** (University of Iowa, USA)

"Enzyme Dynamics and Their Role in Enzyme-Catalyzed Reactions"

8:40 pm - 8:50 pm Discussion

8:50 pm - 9:20 pm **Sharon Hammes-Schiffer** (University of Illinois at Urbana-Champaign, USA)

"Nonadiabatic Dynamics of Photoinduced Proton-Coupled Electron Transfer Processes"

9:20 pm - 9:30 pm Discussion

Tuesday

7:30 am - 8:30 am Breakfast

8:30 am Group Photo

9:00 am - 12:30 pm **Interactions and Dynamics in Materials**

Discussion Leader: **Valeria Kleiman** (University of Florida, USA)

9:00 am - 9:30 am **Tamar Seideman** (Northwestern University, USA)

"Current-Driven Molecular Dynamics in Nanoelectronics"

9:30 am - 9:40 am Discussion

9:40 am - 10:10 am **Alan Aspuru-Guzik** (Harvard University, USA)

"Many-Body Dispersion Effects in the Dynamics and Interactions of Molecules and Two-Dimensional Materials"

10:10 am - 10:20 am Discussion

10:20 am - 10:50 am Coffee Break

10:50 am - 11:20 am **Scott Reid** (Marquette University, USA)

"Dynamics of Excimer Formation in Model Multichromophoric Assemblies"

11:20 am - 11:30 am Discussion

11:30 am - 12:00 pm **Irene Burghardt** (Goethe University Frankfurt, Germany)

"Quantum Dynamics of Excitonic and Charge Transfer Processes in Functional Organic Polymer Materials"

12:00 pm - 12:10 pm Discussion

12:10 pm - 12:25 pm **Heidi Hendrickson** (Yale University, USA)

"Mechanisms for Allosteric Inhibition of Protein Tyrosine Phosphatase 1B"

12:25 pm - 12:30 pm Discussion

12:30 pm Lunch

1:30 pm - 4:00 pm Free Time

4:00 pm - 6:00 pm Poster Session

6:00 pm Dinner

7:30 pm - 9:30 pm **Dynamics and Reactions in Solutions and in Clusters**

Discussion Leader: **Valeria Molinero** (The University of Utah, USA)

7:30 pm - 8:00 pm **Andrew Orr-Ewing** (University of Bristol, United Kingdom)

"Transient Infra-Red Spectroscopy of Solute and Solvent Dynamics for Chemical Reactions in Solution"

8:00 pm - 8:10 pm Discussion

8:10 pm - 8:40 pm **Stephen Bradforth** (University of Southern California, USA)

"Time-Resolving Reactions in Bulk and Interfacial Water with Photoelectron Spectroscopy"

8:40 pm - 8:50 pm Discussion

8:50 pm - 9:20 pm **Hanna Reisler** (University of Southern California, USA)

"Imaging Studies of Photoinitiated Decomposition of Molecules and Clusters"

9:20 pm - 9:30 pm Discussion

Wednesday

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Interfacial Dynamics and Reactions**

Discussion Leader: **David Nesbitt** (JILA, University of Colorado Boulder, USA)

9:00 am - 9:15 am **Sarah King** (Fritz Haber Institute of the Max Planck Society, Germany)

"Dynamics and Reactivity of Trapped Electrons at the Amorphous Solid Water/Vacuum Interface"

9:15 am - 9:20 am Discussion

9:20 am - 9:35 am **Steven Strong** (University of Colorado Boulder, USA)

"The Dynamical Hydrophobic Effect in Nanoporous Graphene"

9:35 am - 9:40 am Discussion

9:40 am - 10:10 am **Ilan Benjamin** (University of California, Santa Cruz, USA)

"Molecular Interactions and Dynamics at the Water/Oil Interface"

10:10 am - 10:20 am Discussion

10:20 am - 10:50 am Coffee Break

10:50 am - 11:20 am **Alec Wodtke** (Max Planck Institute for Biophysical Chemistry, Germany)
"The Influence of Electron Hole Pair Excitation on Adsorption"

11:20 am - 11:30 am Discussion

11:30 am - 12:00 pm **Francesco Paesani** (University of California, San Diego, USA)
"Many-Body Molecular Dynamics: A New Methodology for Computer Simulations with Chemical and Spectroscopic Accuracy of Aqueous Systems from the Gas to the Condensed Phase"

12:00 pm - 12:10 pm Discussion

12:10 pm - 12:25 pm **Marissa Weichman** (University of California, Berkeley, USA)
"Slow Photoelectron Velocity-Map Imaging (SEVI) Spectroscopy of Cryo-Cooled Anions"

12:25 pm - 12:30 pm Discussion

12:30 pm Lunch

1:30 pm - 4:00 pm Free Time

4:00 pm - 6:00 pm Poster Session

6:00 pm Dinner

7:00 pm - 7:30 pm Business Meeting

Nominations for the Next Vice Chair; Fill in Conference Evaluation Forms; Discuss Future Site and Scheduling Preferences; Election of the Next Vice Chair

7:30 pm - 9:30 pm **Unraveling the Dynamics of Catalytic Reactions**

Discussion Leader: **Bruce Kay** (Pacific Northwest National Laboratory, USA)

7:30 pm - 8:00 pm **Tanja Cuk** (University of California, Berkeley, USA)
"Charge Dynamics and Catalytic Intermediates at Solid-Liquid Interfaces"

8:00 pm - 8:10 pm Discussion

8:10 pm - 8:40 pm **Etienne Garand** (University of Wisconsin-Madison, USA)
"Probing Catalytic Reaction Intermediates with Cryogenic Ion Vibrational Spectroscopy"

8:40 pm - 8:50 pm Discussion

8:50 pm - 9:20 pm **Thomas Miller** (California Institute of Technology, USA)
"Computationally Guided Design of Polymer Electrolytes for Battery Applications"

9:20 pm - 9:30 pm Discussion

Thursday

7:30 am - 8:30 am Breakfast

9:00 am - 12:30 pm **Photochemistry and Nonadiabatic Dynamics**

Discussion Leader: **David Yarkony** (Johns Hopkins University, USA)

9:00 am - 9:30 am **David Osborn** (Sandia National Laboratories, USA)

"Photodissociation of Acetylacetone: What Happens When One Molecule Is both a Ketone and an Enol"

9:30 am - 9:40 am Discussion

9:40 am - 10:10 am **Laurie Butler** (University of Chicago, USA)

"Chemical Reaction Dynamics of Radical Intermediates"

10:10 am - 10:20 am Discussion

10:20 am - 10:50 am Coffee Break

10:50 am - 11:20 am **Albert Stolow** (University of Ottawa / National Research Council, Canada)

"Towards Polanyi Rules for Polyatomics: Vibrational Dynamics at Conical Intersections"

11:20 am - 11:30 am Discussion

11:30 am - 12:00 pm **Hua Guo** (University of New Mexico, USA)

"Quantum Non-Adiabatic Dynamics in Photodissociation"

12:00 pm - 12:10 pm Discussion

12:10 pm - 12:25 pm **Kana Takematsu** (Bowdoin College, USA)

"Probing Charge Transfer Processes in Modified Azurin and Aminonaphthol Compounds"

12:25 pm - 12:30 pm Discussion

12:30 pm Lunch

1:30 pm - 4:00 pm Free Time

4:00 pm - 6:00 pm Poster Session

6:00 pm Dinner

7:30 pm - 9:30 pm **Paradigms of Molecular Interactions and Dynamics**

Discussion Leader: **Anne McCoy** (University of Washington, USA)

7:30 pm - 8:00 pm **Stephen Leone** (University of California, Berkeley, USA)

"An X-Ray Spectroscopic Revolution in Time-Resolved Molecular Dynamics"

8:00 pm - 8:10 pm Discussion

8:10 pm - 8:40 pm **Leticia Gonzalez** (University of Vienna, Austria)

"Ultrafast Excited State Dynamics Including Intersystem Crossing. Challenges and Case Studies"

8:40 pm - 8:50 pm Discussion

8:50 pm - 9:20 pm **Richard Zare** (Stanford University, USA)

"All About H2"

9:20 pm - 9:30 pm Discussion

Friday

7:30 am - 8:30 am Breakfast

9:00 am Departure

Molecular Interactions & Dynamics (GRS)

Gordon Research Seminar

New Experimental and Theoretical Techniques for Understanding Energy Transfer and Dynamics of Chemical Reactions

July 9-10, 2016

Stonehill College

Easton, MA

Chairs: [Olga Gorlova](#) & [Mark Shapero](#)

Contributors



The conference also gratefully acknowledges a contribution from Dean and Cindi Guyer.

Meeting Program

Saturday

2:00 pm - 5:00 pm	Arrival and Check-in
3:30 pm - 3:45 pm	Introductory Comments by GRC Site Staff / Welcome by the GRS Conference Chair
3:45 pm - 4:30 pm	Keynote Session: Interactions Between Experiment and Theory Discussion Leader: Mark Shapero (University of California, Berkeley, USA)
3:45 pm - 3:50 pm	Introduction by Discussion Leader
3:50 pm - 4:20 pm	Anne McCoy (University of Washington, USA) "Working at the Crossroads Between Experiment and Theory: Reflections on Conferences, Collaborating and My Career in Chemistry"
4:20 pm - 4:30 pm	Discussion
4:30 pm - 6:00 pm	<u>Poster Session</u>
6:00 pm	Dinner
7:30 pm - 9:30 pm	Biomolecules and Surface Phenomena Discussion Leader: Marissa Weichman (University of California, Berkeley, USA)
7:30 pm - 7:40 pm	Introduction by Discussion Leader
7:40 pm - 7:55 pm	James Davies (Lawrence Berkeley National Laboratory, USA) "Molecular Mobility and Interfacial Chemistry in Aerosol"

- 7:55 pm - 8:00 pm Discussion
- 8:00 pm - 8:15 pm **Andrew Deblase** (Purdue University, USA)
"Conformation-Specific IR and UV Spectroscopy of Cold [YAPAA+H]⁺ Ions: A Stereochemical 'Twist' on the Type II Prime Beta Turn"
- 8:15 pm - 8:20 pm Discussion
- 8:20 pm - 8:35 pm **David Herlihy** (University of California, Berkeley, USA)
"Direct Observation of the Oxyl Radical of Photocatalytic Water Oxidation"
- 8:35 pm - 8:40 pm Discussion
- 8:40 pm - 8:55 pm **Barak Hirshberg** (Hebrew University of Jerusalem, Israel)
"Quantum Vibrational Spectroscopy of Amino Acids Using Classical Separable Potentials"
- 8:55 pm - 9:00 pm Discussion
- 9:00 pm - 9:15 pm **Simon Purcell** (Heriot-Watt University, United Kingdom)
"Use of Reactive O Atom Scattering to Study the Surface Structure of Ionic Liquids"
- 9:15 pm - 9:20 pm Discussion
- 9:20 pm - 9:30 pm General Discussion

Sunday

- 7:30 am - 8:30 am Breakfast
- 9:00 am - 11:00 am **Chemical Interactions and Dynamics**
Discussion Leader: **Sarah King** (Fritz Haber Institute of the Max Planck Society, Germany)
- 9:00 am - 9:10 am Introduction by Discussion Leader
- 9:10 am - 9:25 am **Rebecca Ingle** (University of Bristol, United Kingdom)
"Structure or Dynamics: What Drives Photoproduct Branching at Conical Intersections?"
- 9:25 am - 9:30 am Discussion
- 9:30 am - 9:45 am **Philip Shushkov** (University of Bonn, Germany)
"An Approximate and Analytical Density Functional Method for Large Systems"
- 9:45 am - 9:50 am Discussion
- 9:50 am - 10:05 am **Kristen Zuraski** (University of Southern California, USA)
"Imaging Studies of Small HCl and H₂O Mixed Clusters"
- 10:05 am - 10:10 am Discussion
- 10:10 am - 10:25 am **John Otto** (The University of Chicago, USA)
"Two Dimensional Electronic Spectroscopy of Cavitand Molecular Switch Reveals Dynamics that Limit FRET Efficiency"

10:25 am - 10:30 am Discussion

10:30 am - 10:45 am **Wyatt Merrill** (University of Wisconsin-Madison, USA)

"Dynamics, Trends, and Quantum Yields for CHBrCl₂ Photodissociation"

10:45 am - 10:50 am Discussion

10:50 am - 11:00 am General Discussion

11:00 am - 12:30 pm Poster Session

Coffee will be served in the poster area from 11:00 am - 11:30 am

12:30 pm Lunch

1:30 pm - 2:30 pm **Mentorship Component: Career Panel**

Discussion Leader: **Olga Gorlova** (Yale University, USA)

1:30 pm - 2:30 pm Panel Discussion

"Exploring Various Career Pathways for Upcoming Science Professionals"

- **Anne McCoy** (University of Washington, USA)
- **David Osborn** (Sandia National Laboratories, USA)
- **Gary Weddle** (Fairfield University, USA)
- **Tara Yacovitch** (Aerodyne Research, Inc., USA)

2:30 pm - 3:00 pm Evaluation Period

Fill in GRS Evaluation Forms

3:00 pm Seminar Concludes

Molecular Interactions & Dynamics GRC – Attendee List

Name	Organization	Participation	Status
Acharya, Atanu	University of Southern California	Poster Presenter	Registered
Allison, Thomas K	Stony Brook University	Poster Presenter	Registered
Amarasinghe, Chandika	University of Missouri-Columbia	Poster Presenter	Registered
Annesley, Christopher J	Air Force Research Laboratory	Poster Presenter	Registered
Aschaffenburg, Daniel	University of California, Berkeley	Poster Presenter	Registered
Aspuru-Guzik, Alan	Harvard University	Speaker	Registered
Benitez, Yanice	University of California, San Diego	Poster Presenter	Registered
Benjamin, Ilan	University of California, Santa Cruz	Speaker	Registered
Berman, Michael R	AFOSR	Attendee	Registered
Bhattacharjee, Aditi	University of California, Berkeley	Poster Presenter	Registered
Bjork, Bryce J	JILA / University of Colorado	Poster Presenter	Registered
Bowman, Joel	Emory University	Speaker	Registered
Bradforth, Stephen E	University of Southern California	Speaker	Registered
Buma, Wybren J	University of Amsterdam	Poster Presenter	Registered
Burghardt, Irene	Goethe University Frankfurt	Speaker	Registered
Buthelezi, Thandi M	Wheaton College	Poster Presenter	Registered
Butler, Laurie J	University of Chicago	Speaker	Registered
Caram, Justin R	Massachusetts Institute of Technology	Poster Presenter	Registered
Chang, Bo Y	Seoul National University	Poster Presenter	Registered
Cheatum, Christopher	University of Iowa	Speaker	Registered
Chen, Xihan	UC Berkeley	Poster Presenter	Registered
Chen, Yuning	Stony Brook University	Poster Presenter	Registered
Cuk, Tanja	University of California, Berkeley	Speaker	Registered
Davies, James F	Lawrence Berkeley National Laboratory	Poster Presenter	Registered
Deblase, Andrew F	Purdue University	Poster Presenter	Registered
Denton, Joanna K	Yale University	Poster Presenter	Registered
Dzukan, Laura C	The Ohio State University	Poster Presenter	Registered
Elles, Christopher G	University of Kansas	Poster Presenter	Registered
Fatehi, Shervin	The University of Texas Rio Grande Valley	Poster Presenter	Registered
Garand, Etienne	University of Wisconsin-Madison	Speaker	Registered
Gerber, Benny	University of California, Irvine	Speaker	Registered
Gierster, Lukas	Fritz Haber Institute of the Max Planck Society	Poster Presenter	Registered
Gonzalez, Leticia	University of Vienna	Speaker	Registered
Gorlova, Olga	Yale University	Poster Presenter	Registered
Gunina, Anastasia O	University of Southern California	Poster Presenter	Registered
Guo, Hua	University of New Mexico	Speaker	Registered
Hall, Gregory E	Brookhaven National Laboratory	Poster Presenter	Registered
Hammes-Schiffer, S	University of Illinois at Urbana-Champaign	Speaker	Registered
Hendrickson, Heidi P	Yale University	Speaker	Registered

Herlihy, David M	University of California, Berkeley	Poster Presenter	Registered
Hirshberg, Barak	Hebrew University of Jerusalem	Poster Presenter	Registered
Huang, Wen-Tsung	University of Wisconsin-Madison	Poster Presenter	Registered
Ingle, Rebecca	University of Bristol	Poster Presenter	Registered
Isbill, Sara B	University of Tennessee	Poster Presenter	Registered
Jain, Amber	University of Pennsylvania	Poster Presenter	Registered
Janke, Svenja M	University of Goettingen	Poster Presenter	Registered
Jiang, Hongyan	University Goettingen	Poster Presenter	Registered
Johnson, Mark A	Yale University	Attendee	Registered
Kable, Scott	University of New South Wales	Discussion Leader	Registered
Kaufmann, Sven	Max-Planck-Institute for Biophysical Chemistry	Poster Presenter	Registered
Kay, Bruce D	Pacific Northwest National Laboratory	Discussion Leader	Registered
Kern, Jesse L	University of Tennessee	Poster Presenter	Registered
King, Sarah B	Fritz Haber Institute of the Max Planck Society	Speaker	Registered
Kleiman, Valeria D	University of Florida	Discussion Leader	Registered
Kopplitz, Brent D	Tulane University	Attendee	Registered
Kumar, Gaurav	University of Southern California	Poster Presenter	Registered
Kunin, Alice	UC Berkeley	Poster Presenter	Registered
Kwasniewski, Daniel T	University of Southern California	Poster Presenter	Registered
Le, Nam Q	U.S. Naval Research Laboratory	Poster Presenter	Registered
Lee, Sebastian	California Institute of Technology	Poster Presenter	Registered
Leone, Stephen	University of California, Berkeley	Speaker	Registered
Lester, Marsha I	University of Pennsylvania	Speaker	Registered
Levandier, Dale J	Boston College	Poster Presenter	Registered
Lewandowski, Heather	University of Colorado Boulder	Speaker	Registered
Liu, Yu	Harvard University	Poster Presenter	Registered
Livingston Large, T	JILA-University of Colorado Boulder	Poster Presenter	Registered
Loomis, Richard A	Washington University in St. Louis	Vice Chair	Registered
Lu, Wenchao	Graduate Center of the City University of New York	Poster Presenter	Registered
Lunny, Katharine	University of California, San Diego	Poster Presenter	Registered
Makarem, Camille	Washington University in St. Louis	Poster Presenter	Registered
Marroux, Hugo	University of Bristol	Poster Presenter	Registered
Matsika, Spiridoula	Temple University	Chair	Registered
Mayes, Maricris L	University of Massachusetts Dartmouth	Poster Presenter	Registered
McCoy, Anne B	University of Washington	Discussion Leader	Registered
Medders, Gregory R	University of Pennsylvania	Poster Presenter	Registered
Medina, Jorge I	University of Florida Chemistry	Poster Presenter	Registered
Merrill, Wyatt	University of Wisconsin-Madison	Poster Presenter	Registered
Miller, Thomas F	California Institute of Technology	Speaker	Registered
Mitchell-Koch, Katie R	Wichita State University	Poster Presenter	Registered
Mo, Yuxiang	Tsinghua University	Poster Presenter	Registered

Molinerio, Valeria	University of Utah	Discussion Leader	Registered
Murray, Vanessa	Montana State University	Poster Presenter	Registered
Nathanson, Gilbert M	University of Wisconsin-Madison	Chair	Registered
Ndengue, Steve A	Missouri University of Science and Technology	Poster Presenter	Registered
Nee, Matthew J	Western Kentucky University	Poster Presenter	Registered
Nelson, Daniel	JILA/University of Colorado Boulder	Poster Presenter	Registered
Nesbitt, David J	JILA, University of Colorado Boulder	Discussion Leader	Registered
Ni, Kang-Kuen	Harvard University	Poster Presenter	Registered
Okutsu, Kenichi	Tohoku University	Poster Presenter	Registered
Oliveira, Allan M	JILA - University of Colorado	Poster Presenter	Registered
Oliver, Tom A A	University of Bristol	Attendee	Registered
Opoku-Agyeman, B	The Ohio State University	Poster Presenter	Registered
Orr-Ewing, Andrew	University of Bristol	Speaker	Registered
Osborn, David L	Sandia National Laboratories	Speaker	Registered
Otto, John P	The University of Chicago	Poster Presenter	Registered
Paesani, Francesco	University of California, San Diego	Speaker	Registered
Pal, Partha P	Northwestern University	Poster Presenter	Registered
Peter, Christine	University of Konstanz	Speaker	Registered
Pollock, Kevin L	UC Berkeley	Poster Presenter	Registered
Pratt, David	University of Vermont	Attendee	Registered
Purcell, Simon M	Heriot-Watt University	Poster Presenter	Registered
Qu, Chen	Emory University	Poster Presenter	Registered
Ramasesha, Krupa	Sandia National Laboratories	Poster Presenter	Registered
Reid, Scott A	Marquette University	Speaker	Registered
Reisler, Hanna	University of Southern California	Speaker	Registered
Roy, Sharani	University of Tennessee, Knoxville	Attendee	Registered
Samanta, Bibek R	University of Southern California	Poster Presenter	Registered
Sanyal, Shourjya	University College Dublin	Poster Presenter	Registered
Scrape, Preston G	University of Chicago	Poster Presenter	Registered
Seideman , Tamar	Northwestern University	Speaker	Registered
Shapero, Mark	University of California, Berkeley	Poster Presenter	Registered
Shuman, Nicholas S	Air Force Research Laboratory	Speaker	Registered
Shushkov, Philip G	University of Bonn	Poster Presenter	Registered
Sims, Ian R	University of Rennes 1	Poster Presenter	Registered
Skomorowski, Wojciech	University of Kassel	Speaker	Registered
Smoll, Eric J	Montana State University	Poster Presenter	Registered
Sobyra, Thomas	University of Wisconsin Madison	Poster Presenter	Registered
Sola, Ignacio R	Universidad Complutense	Poster Presenter	Registered
Spata, Vincent A	Temple University	Poster Presenter	Registered
Stolow, Albert	University of Ottawa / National Research Council	Speaker	Registered
Strong, Steven E	University of Colorado Boulder	Speaker	Registered

Sullivan, Erin	University of California Berkeley	Poster Presenter	Registered
Sutradhar, Subhasish	University of Southern California	Poster Presenter	Registered
Takematsu, Kana	Bowdoin College	Speaker	Registered
Tasseven, Cetin	Yildiz Technical University	Poster Presenter	Registered
Thompson, James OF	University of Missouri	Poster Presenter	Registered
Verlet, Jan R	Durham University	Discussion Leader	Registered
Viggiano, Albert A	Air Force Research Laboratory	Attendee	Registered
Wategaonkar, Sanjay	Tata Institute of Fundamental Research	Poster Presenter	Registered
Weeraratna, Chaya	University of Missouri	Poster Presenter	Registered
Wei, Wei	Texas A&M University	Poster Presenter	Registered
Weichman, Marissa L	University of California, Berkeley	Speaker	Registered
Wodtke, Alec	Max Planck Institute for Biophysical Chemistry	Speaker	Registered
Xantheas, Sotiris S	Pacific Northwest National Laboratory	Speaker	Registered
Xu, Hong	Brookhaven National Laboratory	Poster Presenter	Registered
Yang, Xueming	Dalian Institute of Chemical Physics	Speaker	Registered
Yarkony, David R	Johns Hopkins University	Discussion Leader	Registered
Yu, Qi	Emory University	Poster Presenter	Registered
Zare, Richard	Stanford University	Speaker	Registered
Zobel, Patrick	University of Vienna	Poster Presenter	Registered
Zuraski, Kristen L	University of Southern California	Poster Presenter	Registered
Zwier, Timothy S	Purdue University	Discussion Leader	Registered

Molecular Interactions & Dynamics GRS – Attendee List

Name	Organization	Participation	Status
Acharya, Atanu	University of Southern California	Poster Presenter	Registered
Benitez, Yanice	University of California, San Diego	Poster Presenter	Registered
Bhattacharjee, Aditi	University of California, Berkeley	Poster Presenter	Registered
Chen, Xihan	UC Berkeley	Poster Presenter	Registered
Chen, Yuning	Stony Brook University	Poster Presenter	Registered
Davies, James F	Lawrence Berkeley National Laboratory	Speaker	Registered
Deblase, Andrew F	Purdue University	Speaker	Registered
Denton, Joanna K	Yale University	Poster Presenter	Registered
Dzugas, Laura C	The Ohio State University	Poster Presenter	Registered
Gierster, Lukas	Fritz Haber Institute of the Max Planck Society	Poster Presenter	Registered
Gorlova, Olga	Yale University	Chair	Registered
Gunina, Anastasia O	University of Southern California	Poster Presenter	Registered
Hendrickson, Heidi P	Yale University	Poster Presenter	Registered
Herlihy, David M	University of California, Berkeley	Speaker	Registered
Hirshberg, Barak	Hebrew University of Jerusalem	Speaker	Registered
Huang, Wen-Tsung	University of Wisconsin-Madison	Poster Presenter	Registered
Ingle, Rebecca	University of Bristol	Speaker	Registered
Isbill, Sara B	University of Tennessee	Poster Presenter	Registered
Jain, Amber	University of Pennsylvania	Poster Presenter	Registered
Janke, Svenja M	University of Goettingen	Poster Presenter	Registered
Jiang, Hongyan	University Goettingen	Poster Presenter	Registered
Kaufmann, Sven	Max-Planck-Institute for Biophysical Chemistry	Poster Presenter	Registered
King, Sarah B	Fritz Haber Institute of the Max Planck Society	Discussion Leader	Registered
Kumar, Gaurav	University of Southern California	Poster Presenter	Registered
Kunin, Alice	UC Berkeley	Poster Presenter	Registered
Kwasniewski, Daniel T	University of Southern California	Poster Presenter	Registered
Le, Nam Q	U.S. Naval Research Laboratory	Poster Presenter	Registered
Liu, Yu	Harvard University	Poster Presenter	Registered
Lunny, Katharine	University of California, San Diego	Poster Presenter	Registered
Makarem, Camille	Washington University in St. Louis	Poster Presenter	Registered
Marroux, Hugo	University of Bristol	Poster Presenter	Registered
McCoy, Anne B	University of Washington	Speaker	Registered
Medders, Gregory R	University of Pennsylvania	Poster Presenter	Registered
Medina, Jorge I	University of Florida Chemistry	Poster Presenter	Registered
Merrill, Wyatt	University of Wisconsin-Madison	Speaker	Registered
Murray, Vanessa	Montana State University	Poster Presenter	Registered
Ndengue, Steve A	Missouri University of Science and Technology	Poster Presenter	Registered
Oliveira, Allan M	JILA - University of Colorado	Poster Presenter	Registered
Opoku-Agyeman, B	The Ohio State University	Poster Presenter	Registered

Osborn, David L	Sandia National Laboratories	Speaker	Registered
Otto, John P	The University of Chicago	Speaker	Registered
Pollock, Kevin L	UC Berkeley	Poster Presenter	Registered
Purcell, Simon M	Heriot-Watt University	Speaker	Registered
Qu, Chen	Emory University	Poster Presenter	Registered
Samanta, Bibek R	Univeristy of Southern California	Poster Presenter	Registered
Scrape, Preston G	University of Chicago	Poster Presenter	Registered
Shapero, Mark	University of California, Berkeley	Chair	Registered
Shushkov, Philip G	University of Bonn	Speaker	Registered
Skomorowski, W	University of Kassel	Poster Presenter	Registered
Smoll, Eric J	Montana State University	Poster Presenter	Registered
Sobyra, Thomas	University of Wisconsin Madison	Poster Presenter	Registered
Spata, Vincent A	Temple University	Poster Presenter	Registered
Strong, Steven E	University of Colorado Boulder	Poster Presenter	Registered
Sullivan, Erin	University of California Berkeley	Poster Presenter	Registered
Sutradhar, Subhasish	University of Southern California	Poster Presenter	Registered
Weddle, Gary H	Fairfield University	Speaker	Registered
Weichman, Marissa L	University of California, Berkeley	Discussion Leader	Registered
Yacovitch, Tara I	Aerodyne Research, Inc.	Speaker	Registered
Zobel, Patrick	University of Vienna	Poster Presenter	Registered
Zuraski, Kristen L	University of Southern California	Speaker	Registered