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University of Florida - Gainesville
219 Grinter Hall
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RPPR Final Report
as of 16-Oct-2018

Agency Code:

Proposal Number: 70861CHCF **Agreement Number: W911NF-17-1-0041**
INVESTIGATOR(S):

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DUNS Number: 969663814 EIN: 596002052
Report Date: 31-Mar-2018 Date Received: 11-Oct-2018
Final Report for Period Beginning 01-Jan-2017 and Ending 31-Dec-2017
Title: 57th Sanibel Symposium: The Theory Meeting for Theoreticians!
Begin Performance Period: 01-Jan-2017 **End Performance Period:** 31-Dec-2017
Report Term: 0-Other
Submitted By: Rodney Bartlett Email: bartlett@qtp.ufl.edu
Phone: (352) 392-6974
Distribution Statement: 1-Approved for public release; distribution is unlimited.

STEM Degrees: **STEM Participants:**

Major Goals: Support 57th Sanibel Symposium

Accomplishments: The 57th Sanibel Symposium organized by the University of Florida's Quantum Theory Project was held from February 19th, 2017 to February 24th, 2017 at the King and Prince Resort at St. Simon Island, GA. The conference celebrated the Science of the late Nobel prize winner, Walter Kohn, emphasizing his work on Density Functional Theory. In addition the symposium celebrated the 50th Anniversary of Ji?í ?ížek's paper that started coupled-cluster theory, today's
per-eminent ab initio approach to the electronic structure of molecules.

Training Opportunities: Nothing to Report

Results Dissemination: Proceedings of the 57th Sanibel Meeting will be published in Molecular Physics

Honors and Awards: Nothing to Report

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

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

RPPR Final Report
as of 16-Oct-2018

FINAL REPORT, ARO W911NF-17-1-0041

FOR THE SUPPORT OF THE 57TH SANIBEL MEETING

Rodney Bartlett (PI)

University of Florida

(01/01/2017 – 12/31/2017)

The 57th Sanibel Symposium organized by the University of Florida's Quantum Theory Project was held from February 19th, 2017 to February 24th, 2017 at the King and Prince Resort at St. Simon Island, GA. The conference celebrated the Science of the late Nobel prize winner, Walter Kohn, emphasizing his work on Density Functional Theory. In addition the symposium celebrated the 50th Anniversary of Jiří Čížek's paper that started coupled-cluster theory, today's per-eminent *ab initio* approach to the electronic structure of molecules.

The conference included 33 lectures presented in 9 plenary and 6 invited sessions, subdivided into 15 different topics to cover a variety of state-of-the art work. In addition 33 'hot topic' oral presentations were assigned on a competitive basis from submitted abstracts. All of the plenary, invited, and hot-topic talks were further augmented by five poster presentations of 105 talks. This enables all the attendees to present their results to the expert Sanibel audience in the best format for them.

The total attendance of 210 scientists included 40 Graduate Students. We were particularly pleased with their participation. The ARO sponsorship of $15K is instrumental in making it possible for graduate students to attend the meeting, as it covers their fees among other charges. Attending a conference is a professionally rewarding experience, and the Sanibel

meeting remains the largest, annual meeting in the field. In addition to networking with colleagues from other institutions the scholars and academics annually continue their fertile discussions about the newest developments in the field of the electronic structure of atoms molecules, and solids, and their biochemical applications.

The ARO funds were distributed as follows:

Registration fee support for the Graduate Students and PostDocs	$11,510.06
Travel Awards for Graduate Students and PostDocs	$3,489.94
Total	$15,000.00

The enclosed copies of the program can be consulted for further details of the meeting. In addition, a Proceedings of the 57th Sanibel Meeting will be published in Molecular Physics.

57th Sanibel Symposium

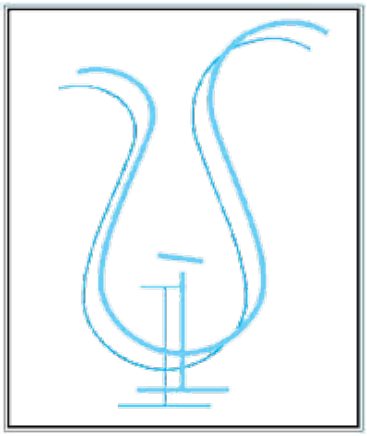
February 19-24, 2017

**King and Prince,
St. Simons Island,
GA, USA**

57th SANIBEL SYMPOSIUM (2017) PLENARY / INVITED / ORAL / POSTER SCHEDULE

Sunday Times	Sunday 2/19	Weekday Times	Monday 2/20	Tuesday 2/21	Wednesday 2/22	Thursday 2/23	Friday 2/24
		8:30 AM	**PLENARY 2**	**PLENARY 3**	**PLENARY 4**	**PLENARY 5**	**PLENARY 9**
			New Developments in Density Functional Theory	***Molecular and Electronic Dynamics***	***Density Functional Theory Including van der Waals Forces***	***Quantum Materials and Spectroscopy***	***Core Excitation Spectroscopy***
			CHAIR: N. Roesch	**CHAIR:** E. de Prince	**CHAIR:** D. Cremer	**CHAIR:** N. Marom	**CHAIR:** J. Stanton
		8:30- 9:10 AM	Xavier Gonze	Rigoberto Hernandez	Timo Thonhauser	Thomas Maier	Nicholas Besley
		9:10 - 9:50 AM	Alex Borgoo	Tammie Nelson	Alexander Tkatchenko	Thomas Peter Devereaux	Lan Cheng
		9:50 - 10:30 AM	Donald Truhlar	David Coker	Gerit Brandenburg	Warren E. Pickett	Sonia Coriani
		10:30 - 10:50 AM	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break
		10:50 AM	**INVITED 2**	**INVITED 3**	**INVITED 4**	**PLENARY 6**	**INVITED 5**
			Kohn-Korringa-Rostoker	***Density Functional Theory in Solids***	***Many-Electron Theory of Molecular Interactions***	***Complex and Functional Materials***	***Fifty Year Anniversary of Jiří Čížek Paper***
			CHAIR: S. Pantelides	**CHAIR:** R. Hennig	**CHAIR:** E. Kraka	**CHAIR:** X. Zhang	**CHAIR:** R. Bartlett
		10:50 - 11:20 AM	William Butler	Mira Todorova	Maria Pilar de Lara-Castells	Lin-Wang Wang	Josef Paldus (11:00am - 11:30am)
		11:20 - 11:50 AM	Hubert Ebert	Christoph Freysoldt	Krzysztof Szalewicz	Janice Musfeldt	Piotr Piecuch (11:30am - 11:50am)
12:00 PM	**Symposium Registration Starts**	11:50 - 12:20 PM	Duane Johnson	Tim Mueller	Jordan R Schmidt	De-En Jiang	Miroslav Urban (11:50am - 12:10pm)
		12:20 - 12:50 PM	Malcolm Stocks	Matthias Rupp	Ilya G. Kaplan	Break for Lunch	John Stanton (12:10pm - 12:30pm)
						(12:30pm - 2:00pm)	Jozef Noga (12:30pm - 12:50pm)
		1:00 PM	Break for Lunch	Break for Lunch	Break for Lunch		Break for Lunch
						PLENARY 7	
2:00 PM	**PLENARY 1**	2:30 PM	**Selected Hot-Topic Talks 1**	**Selected Hot-Topic Talks 2**	**Selected Hot-Topic Talks 3**	***Machine Learning and Algorithms***	**INVITED 6**
	A Celebration of the Science of Walter Kohn		**CHAIR:** F. Harris	**CHAIR:** J. Murray	**CHAIR:** P. Seybold	**CHAIR:** S. Trickey	***Coupled-cluster Theory and the Future***
	CHAIR: B. Kirtman	2:30 - 2:45 PM	Richard Squire	Dillon Scofield	Elvira Sayfutyarova	Kieron Burke (2:00pm - 2:40pm)	**CHAIR:** A. Perera
2:15 - 2:55 PM	Eberhard Gross	2:45 - 3:00 PM	Elfi Kraka	Luis Rincon	Ulises Miranda	Aldo Romero (2:40pm - 3:20pm)	Henry F. Schaefer (2:30pm - 2:50pm)
2:55 - 3:35 PM	Andreas Görling	3:00 - 3:15 PM	Thomas Jagau	Dieter Cremer	Andrew Mahler	John Herbert (3:20pm - 4:00pm)	Mihály Kállay (2:50pm - 3:10pm)
3:35 - 4:15 PM	Paola Gori Giorgi	3:15 - 3:30 PM	Toru Saito	Xiangguo Li	Hemanadhan Myneni	Coffee Break (4:00pm - 4:15pm)	Krzysztof Szalewicz (3:10pm - 3:30pm)
	Coffee Break	3:30 - 3:45 PM	Arkajyoti Sengupta	Mark Iron	Eugene DePrince	**PLENARY 8**	Karol Kowalski (3:30pm - 3:50pm)
4:15 - 4:30 PM	**INVITED 1**	3:45 - 4:00 PM	Arindam Chakraborty	Yun-Peng Wang	José L. Gázquez	***Synthesis and High Throughput***	Daniel Kats (3:50pm - 4:10pm)
	Density Functional Theory	4:00 - 4:15 PM	Xiaopeng Wang	Olaseni Sode	Susi Lehtola	**CHAIR:** J. Greer	Steve Gwaltney (4:10pm - 4:30pm)
	CHAIR: V. Ortiz	4:15 - 4:30 PM	James Dufty	Kieu My Bui	Robert Topper	Shyue Ping Ong (4:15pm - 4:55pm)	Coffee Break (4:30pm - 4:45pm)
4:30 - 5:00 PM	Aron Cohen	4:30 - 4:45 PM	Jesse Lutz	Lan Tran	Dane Hogoboom	Hai-Ping Cheng (4:55pm - 5:35pm)	Monika Musial (4:45pm - 5:05pm)
5:00 - 5:30 PM	Lucian Constantin	4:45 - 5:00 PM	Samuel Brown	Alexander Rusakov	Markus Eisenbach		Sourav Pal (5:05pm - 5:25pm)
5:30 - 6:00 PM	Troy Van Voorhis	5:00 - 5:15 PM	Koichi Yamashita	Jim Greer	Jorge Seminario		Dmitry Lyakh (5:25pm - 5:45pm)
6:00 - 6:30 PM		5:15 PM	**POSTER ONE***	**POSTER THREE***	**POSTER FIVE***	**Cocktail Hour 6:00pm-7:00pm**	Peter Szalay (5:45pm - 6:05pm)
						Hotel Lawn	So Hirata (6:05pm - 6:25pm)
9:00 PM	**Reception**	7:15 PM				**BANQUET**	
	9 PM Delegal Room					7:00 PM Delegal Room	
		9:00 PM	**POSTER TWO***	**POSTER FOUR***		Undergraduate Award	
						Graduate Award	**SYMPOSIUM CONCLUDES**
						Postdoc Award	Cake Reception and Champagne 6:30pm, Retreat Room
11:00 PM		11:00 PM	* Retreat Room			Young Investigator Award	

57TH SANIBEL SYMPOSIUM



SPONSORS:

University of Florida Office of Research

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Quantum Theory Project

AWARDS:

Dell-Intel
Löwdin

IBM-Zerner
Young Investigator

FEBRUARY 19-24, 2017
THE KING AND PRINCE, ST. SIMONS ISLAND, GA, USA

Table of Contents

Program

All Plenary and Invited Sessions will be held in the Lanier Ballroom. All Poster Sessions will be held in the Retreat Room.

Reception
Delegal Room 9:00pm-11:00pm
Two complimentary drink tickets will be provided

Program Continued

Welcome

The 57th Symposium will address several topics primed for critical future development. In addition, to recognize and honor the scientific legacy of Walter Kohn, the meeting will begin with a Sunday afternoon session with several world-famous theorists speaking. Sanibel continues to be known as "The Theory Meeting for Theoreticians." It provides an opportunity for scholars and academics to continue to discuss the newest developments in topic areas and share the latest research endeavors in the field.

Plenary and Invited sessions will cover important progress in the core areas of Electronic Structure Theory. In addition to poster presentations, the new Sanibel format allows for up to thirty-three 15-minute oral presentations, assigned on a hot-topic basis, in order to allow more opportunity for collaborative learning and discussion among Symposium attendees.

All attendees are encouraged to submit papers to the Sanibel Proceedings, published by Molecular Physics (http://www.qtp.ufl.edu/sanibel/proceed.shtml). Over the years, the Sanibel Proceedings have enjoyed an attractive impact factor, as many of the first papers in now well-known developments appeared there, and each year there are new candidates.

The 57th Sanibel Symposium is Sponsored by:

University of Florida Office of Research

United States Army Research Office

United States Department of Energy

Awards:

Dell-Intel IBM-Zerner

Löwdin

Young Investigator

Proceedings Publisher:

Taylor and Francis

General Information

Dates
Sunday, February 19 - Friday, February 24, 2017

Symposium Location

The King and Prince
201 Arnold Road
St. Simons Island, Georgia 31522
1-912-638-3631

Registration Information

Regular Symposium registration includes admission to all scheduled speaker talks, poster sessions, Sunday Reception, breakfast, morning and afternoon beverage breaks, the Banquet Dinner on Thursday night, and the Friday evening Reception. All other meals are on your own; lunch and dinner (excluding Thursday night's Banquet) for each day are not provided to Symposium attendees. One-day registration does not include the Thursday Banquet.

Listed below are the Symposium Registration hours for each day of the Symposium.

Sunday, February 19th: 12:00pm-7:00pm
Monday, February 20th: 8:00am-5:00pm
Tuesday, February 21st: 8:00am-5:00pm
Wednesday, February 22nd: 8:00am-3:00pm
Thursday, February 23rd: 8:00am-5:30pm
Friday, February 24th: 8:00am-1:00pm

Procedures and Practical Matters

Please wear your name badge to all Symposium sessions and events.

Instructions for speakers, poster presenters, and those wishing to contribute to the Proceedings are found on the following page.

Please make special note of the speaker timer instructions. Speakers are required to keep strictly to the allotted time schedule. Failure to adhere to the scheduled speaker times will result in an undue burden on the Session Chair and ultimately deprives subsequent speakers of their rightful alloted speaking time.

Assistance

Questions or requests for assistance can be addressed by the following individuals based on topic category:

Symposium Registration & Poster Sessions
Galyna Vakulenko

Hotel Registration
Hotel Desk

Proceedings
Dr. Rodney Bartlett

Social Activities

Social functions are included in the Registration Fee and are also open to registrants' guests for whom a banquet ticket has been purchased. There are three scheduled social events:

Sunday Evening - Opening Reception

9:00pm to 11:00pm - The Opening Reception will take place in the Delegal Room. Join us for light hors d'oeuvres, desserts, and 2 complimentary glasses of wine, beer, or soft drinks. A cash bar will also be available for attendees wishing to purchase additional beverages.

Thursday Evening - Symposium Banquet

6:00pm-7:00pm - 2 complimentary glasses of wine, beer, or soft drinks will be served on the hotel lawn outside of the Delegal Room (weather permitting). In the event of inclement weather, the cocktail hour will be moved inside to the colonnade, located next to the Delegal Room.

7:00pm-10:00pm - Dinner will be served in the Delegal Room. In addition to the banquet dinner, there will be a presentation of awards. To indicate your choice of menu, please display your colored meal preference coupon.

Friday Evening - Cake and Champagne Reception

6:30pm-8:30pm - Close out the Symposium week with dessert and champagne in the Retreat Room. This is an opportunity for relaxed discussion as we end the 57th Symposium.

Dressy casual attire is suggested for all Symposium social events. For more information regarding Symposium social events, please visit the registration desk.

General Information

Speaker Instructions

All speakers must observe the specified time allotted for their contribution.

- Plenary Speakers- 35 minutes plus 5 minutes for questions
- Invited Speakers- 25 minutes plus 5 minutes for questions
- Oral Contributed Speakers- 12 minutes plus 3 minutes for questions.

A speaker timer will be used to help monitor speaker times:

- The speaker timer will start with a GREEN light.
- The timer will display a YELLOW light when 3 minutes remain of the allotted time.
- The timer will display a RED light when the allotted speaking time is up. At this time, each speaker should allow questions from the audience.

It is preferable for each speaker to finish one to two minutes early to encourage more discussion during the allotted presentation.

Please ask any questions about allocated speaking times at the Symposium registration desk.

The organizers thank the speakers in advance for their participation and for contributing to the success of the 57th Sanibel Symposium

Abstract Access

All abstracts for the 57th Sanibel Symposium can be viewed and downloaded from the "Abstract" tab on the Symposium website www.qtp.ufl.edu/sanibel/abstracts.html

Abstracts from prior year Symposia are accessible under the "Sanibel's History" block on the Symposium home page.

Poster Session Instructions

The poster sessions at the Sanibel Symposium are an essential part of the meeting, as they offer an opportunity for the exchange of forefront ideas. All poster sessions will be held in the Retreat Room.

Each poster contribution consists of an abstract title and presenter's name published in the program, the abstract published online, and the bulletin-board presentation itself. In addition, a manuscript may be submitted to be considered for the Proceedings.

Posters may be placed on the boards provided in the Retreat Room prior to the start of the poster session. Push pins will be available for each presenter to utilize. Poster boards are numbered to correspond with the number next to the presenter's name, as listed in the Symposium schedule under the scheduled day and time. Please remove your poster immediately upon the conclusion of your poster session, so that the presenters in the next poster session have ample time to prepare.

Proceedings Contributions Instructions

Only talks or posters presented at the 2017 Sanibel Symposium are eligible to be submitted to the proceedings issue of Molecular Physics. To ensure rapid publication of the Proceedings, contributors are expected to submit completed manuscripts to Molecular Physics electronically. Submission must be completed by April 30, 2017. The instructions for submissions can be found at http://mc.mauscriptcentral.com/tmph. Please create an account (if you do not already have one), and log on to the author center. The editor of the Sanibel Proceedings is Dr. Rodney Bartlett. All manuscripts will be refereed according to the standard rules of Molecular Physics. Refereeing will be electronic and accessible from the same site.

Symposium attendees are welcome to access the 2017 Sanibel Symposium proceedings online. The free content will be accessible via http://www.tandfonline.com/r/tmph-113-3-4. The user will be prompted to sign in or register with Taylor & Francis Online before gaining access to the online proceedings.

General Information

Organizing Staff

Symposium Organizers:

Rodney J. Bartlett

Hai-Ping Cheng

Erik Deumens

Frank E. Harris

Richard Hennig

Ajith Perera

Simon Phillpot

Samuel B. Trickey

Xiaoguang Zhang

Other QTP Members:

David A. Micha

Hendrik Monkhorst

N. Yngve Öhrn

John R. Sabin

Beverly A. Sanders

Symposium Coordinator:

Galyna Vakulenko
University of Florida, Chemistry Department

Proceedings Editor:

Rodney J. Bartlett

Sanibel Symposium Endowment

The longevity of the Sanibel Symposium's engagement of international scientists in atomic, molecular, biomolecular, and condensed matter theory and computation demonstrates the important role of the meeting. Since the first Sanibel Symposium (arranged by Per-Olov Löwdin in January 1961 on Sanibel Island in the Gulf of Mexico) over 5,000 scientists have participated. From 1978 until 2004, the Sanibel Symposium was hosted in several locations on or near the Atlantic Ocean. Since 2005, the Symposium has been held at The King and Prince on St. Simons Island, Georgia.

Federal agencies, foundations, industrial sponsors, and the University of Florida have made it possible to arrange a compelling, up-to-date Symposium each year. However, the continued funding of the meeting is of concern. The organizers and the faculty and staff of QTP have worked diligently toward a more stable and independent financial base for the Sanibel Symposium. An endowment was established to support the meeting. The endowment is an essential part of the effort needed to secure the continuing support of the meeting and to encourage participation of young scientists.

In contrast to endowments for building of athletic programs, the Sanibel Endowment serves as a support of intellectual pursuits. It must be borne by relatively small numbers of individuals and organizations who understand the value of those pursuits. Therefore, we turn to you with this appeal to solicit a gift for the endowment.

Levels of Support:

$10,000- Symposium Patron

$5,000-$9,999- Symposium Donor

$1,000-$4,999- Symposium Supporter

We emphasize that any level of support is most welcome. Your gift may be tax deductible.

Please make your check payable to the University of Florida Foundation, Sanibel Symposia Endowment Fund and mail to:

Rod Bartlett, Director
University of Florida/ QTP
P.O. Box 118435
Gainesville, FL 32611

We thank the following colleagues and friends for their generous contributions to the Sanibel Endowment Fund

Symposium Patrons

IBM

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Mr. Christopher J. Obara

Dr. Otto E. Steinborn

Dr. J. Patrick Tatum

Sunday, February 19, 2017

Plenary 1 - A Celebration of the Science of Walter Kohn
2:00pm-3:15pm

Chair: Bernard Kirtman *University of California Santa Barbara*

Eberhard Gross *MPI for Microstructure Physics*

Walter Kohn: The Science and the Man

Andreas Görling *University Erlangen-Nuremberg*

Power series approximation for the correlation kernel leading to Kohn-Sham methods combining accuracy, computational efficiency, and general applicability

Paola Gori-Giorgi *Vrije Universiteit Amsterdam*

Exchange-Correlation functionals inspired to the exact strong coupling limit of density functional theory

Invited 1 - Density Functional Theory
3:30pm-6:50pm

Chair: Vincent Ortiz *Auburn University*

Aron Cohen *University of Cambridge*

The exact functional of density functional theory

Lucian Constantin *Italian Institute of Technology*

Semiclassical atom theory applied to solid-state physics

Troy Van Voorhis *Massachusetts Institute of Technology*

The Many Pair Expansion: a density functional hierarchy for correlation

Monday, February 20, 2017

Plenary 2 - New Developments in Density Functional Theory
8:30am-10:30am

Chair: Notker Rösch *Technische Universität München*

Xavier Gonze *Université Catholique de Louvain*

Electronic structure of solids, including vibrational effects : Temperature dependence and zero-point motion

Alex Borgoo *University of Oslo*

Excitation energies from the time-independent ensemble Density-Functional Theory

Donald Truhlar *University of Minnesota*

Recent advances in Kohn-Sham density functional theory and multiconfiguration pair-density functional theory

Monday, February 20, 2017

Invited 2- Kohn-Korringa-Rostoker
10:50am-12:50pm

Chair: Sokrates Pantelides *Vanderbilt University*

William Butler *University of Alabama*

Korringa-Kohn-Rostoker approach to band theory

Hubert Ebert *Ludwig Maximilian University of Munich*

Transport properties calculated by means of the Kubo formalism and using the spin-polarized relativistic KKR-CPA method

Duane Johnson *Iowa State University/Ames Laboratory*

From high-entropy alloys to warm-dense matter in a single framework: thermodynamic properties from KKR multiple-scattering theory

Malcolm Stocks *Oak Ridge National Laboratory*

Korringa-Kohn-Rostoker electronic structure theory 50 years on "understanding the physical properties of concentrated solid solution and high entropy alloys"

Selected Hot-Topic Talks 1
2:30pm-5:00pm

Chair: Frank Harris *University of Florida*

Richard Squire *Institute of Technology - West Virginia University*

Coherent ground and excited states permit nearly perfect energy transfer in the B850 / B875 photosynthetic complex in rhodopseudomonas acidophila bacteria

Elfi Kraka *Southern Methodist University*

The secrets of gold catalysis

Thomas Jagau *Ludwig Maximilian University of Munich*

Analytic gradients for the complex absorbing potential equation-of-motion coupled-cluster method

Toru Saito *Osaka University*

Reparameterization of PM6 applied to through-bond and through-space magnetic interactions

Arkajyoti Sengupta *Indiana University*

Connectivity-based hierarchy (CBH): a route to highly accurate reaction enthalpies of organic reactions with cheap DFT methods

Arindam Chakraborty *Syracuse University*

Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states

Xiaopeng Wang *Carnegie Mellon University*

Effect of crystal packing on the excitonic properties of rubrene polymorphs

James Dufty *University of Florida*

Development and applications of orbital free density functional theory

Olaseni Sode *University of Tampa*

Development of a "first principles" carbon dioxide potential and its application to clusters up to $(CO_2)_{13}$

Monday, February 20, 2017

Selected Hot-Topic Talks 1 - Continued
2:30pm-5:00pm

Chair: Frank Harris *University of Florida*

Samuel Brown *North Dakota State University*

Exploring the oxidation states of optically active silver nanoclusters for biological applications

Koichi Yamashita *The University of Tokyo*

Structural and electronic features of hybrid organic–inorganic halide perovskite clusters and surfaces: insights from first principles

Poster 1
5:00pm-7:00pm

1 - Alex Bazante *University of Florida*

Core excitation spectra in attosecond spectroscopy: a coupled cluster study of FCl

2 - Joanna Bednarska *Wroclaw University of Science and Technology*

On the performance of exchange-correlation functionals in the calculations of vibrational reorganization energy

3 - Daniel Chaves Claudino *University of Florida*

Dimer-based atomic basis sets from coupled-cluster theory

4 - Jun Jiang *University of Florida*

Nonradiative hot carrier capture cross section of defects in GaN from first principles

5 - Yifan Jin *University of Florida*

Making the Kohn-Sham density functional theory to converge to the right answer

6 - Ryo Kiribayashi *Hiroshima City University*

Molecular dynamics study of the structural stability of CDR-H3 of anti-HIV neutralizing antibody PG16

7 - Lukas Konecny *Comenius University in Bratislava*

Calculation of molecular properties from relativistic electron dynamics

8 - Shubin Liu *University of North Carolina*

Electronic forces as descriptors of nucleophilic and electrophilic regioselectivity and stereoselectivity

9 - Johannes Margraf *University of Florida*

Correlated orbital approximations: properties of semiempirical correlation potentials

10 - Yuki Mitsuta *Osaka University*

The algorithm of automatic umbrella sampling with umbrella integration

11 - Satoshi Nakagawa *Kanazawa University*

Theoretical study on intermolecular interaction and structural stability of plastocyanin and cytochrome f complex by using the Go-like model

Poster 1 - Continued
5:00pm-7:00pm

12 - Youngchoon Park *University of Florida*

A numerically stable ΔSCF-DFT from constricted variational density functional theory: theory and calculation for triplet states

13 - Duminda Ranasinghe *University of Florida*

Does the ionization potential condition employed in QTP functionals mitigate the self-interaction error?

14 - Paul G. Seybold *Wright State University*

A stochastic cellular automata model of tautomer equilibria

15 - D. Jonathan Vogel *University of South Dakota*

Role of lead vacancies for optoelectronic properties of lead-halide perovskites

Poster 2
9:00pm-11:00pm

1 - Marta Choluj *Wroclaw University of Science and Technology*

On the electronic and vibrational contributions to the static electric properties of molecular complexes under spatial confinement

2 - Marc Coons *Ohio State University*

Energetics of solvated ions and the hydrated electron in bulk water and at a water-vapor interface

3 - Adam Erck *University of South Dakota*

Computationally-supported metal organic super container discovery

4 - Takeshi Iwasa *Hokkaido University*

A theoretical method for infrared absorption spectroscopy based on the multipolar hamiltonian

5 - Muneaki Kamiya *Gifu University*

Ab initio excited-state molecular dynamics approach including spin-orbit coupling and nonadiabatic coupling effects: an application to the photodissociation of CH_3I

6 - Megumi Kayanuma *University of Tsukuba*

A theoretical study of glycine formation reactions in interstellar medium

7 - Elvis Maradzike *Florida State University*

Analytic gradients for v2RDM-CASSCF methods

8 - Michael Metz *University of Delaware*

Automatic generation of intermolecular potential energy surfaces

9 - David Micha *University of Florida*

Photoabsorbance of supported metal clusters: Ab initio density matrix and model studies of large Ag clusters on Si surfaces

Monday, February 20, 2017

Poster 2 - Continued
9:00pm-11:00pm

10 - Wayne Mullinax *Florida State University*

Efficient implementation of a large-scale v2RDM-driven CASSCF method

11 - Tomoki Nakayoshi *Kanazawa University*

A computational study of racemization mechanism of aspartate residue catalyzed by phosphate ion

12 - Daniel Nascimento *Florida State University*

Linear absorption spectroscopy from explicitly time-dependent equation-of-motion coupled cluster theory

13 - Tetsuya Taketsugu *Hokkaido University*

AIMD study on ππ-excited substituted-stilbene*

14 - Kizashi Yamaguchi *Riken Advanced Institute for Computational Science*

Double hybrid density functional calculations of the $CaMn_4O_5$ cluster in the S_3 state of oxygen evolving complex in photosystem II

Tuesday, February 21, 2017

Plenary 3 - Molecular and Electronic Dynamics
8:30am-10:30am

Chair: Eugene de Prince *Florida State University*

Rigoberto Hernandez *Johns Hopkins University*

Coarse-graining solvent structure using stochastic hard collision (SHC) dynamics

Tammie Nelson *Los Alamos National Lab*

Efficient nonadiabatic excited-state molecular dynamics simulations for large molecules

David Coker *Boston University*

First principles model hamiltonian ensembles and quantum dynamics for photosynthetic light harvesting

INVITED 3 - DENSITY FUNCTIONAL THEORY IN SOLIDS
10:50AM-12:50PM

Chair: Richard Hennig *University of Florida*

Mira Todorova *Max-Planck-Institut für Eisenforschung*

From semiconductor defect chemistry to electrochemistry: Insights into corrosion mechanisms from ab initio concepts

Christoph Freysoldt *Max-Planck-Institut für Eisenforschung*

Ab initio simulations of charged surfaces

Tim Mueller *Johns Hopkins University*

The effective use of data in materials research

Matthias Rupp *Fritz Haber Institute of the Max Planck Society*

Many-body tensor representation for machine learning of solids

SELECTED HOT-TOPIC TALKS 2
2:30PM-5:00PM

Chair: Jane Murray *University of New Orleans*

Dillon Scofield *Oklahoma State University*

Implications of causality for quantum biology

Jesse Lutz *Air Force Institute of Technology*

Performance of the two-determinant coupled-cluster method for triplet and open-shell singlet states of biradical molecules

Dieter Cremer *Southern Methodist University*

Development and application of Dirac-exact relativistic methods: second-order response properties

Xiangguo Li *University of Florida*

First-principles study of graphene/transition metal dichalcogenide/graphene field-effect transistors

Mark Iron *Weizmann Institute of Science*

Factors impacting the accuracy of 13C NMR chemical shift predictions using density functional theory – the advantage of long-range corrected functionals

Yun-Peng Wang *University of Florida*

First-principles studies of ferroelectricity in $BiMnO_3$ thin films

Susi Lehtola *Lawrence Berkeley National Laboratory*

Cost-effective description of strong correlation via the perfect pairing hierarchy

Kieu My Bui *University of Tsukuba*

First principle analysis of ammonia adsorption and desorption on GaN surface

Lan Tran *University of Michigan*

Ab initio self-energy embedding theory for realistic systems

Alexander Rusakov *University of Michigan*

Electronic correlations in solids via finite-temperature Green's functions

Jim Greer *Tyndall National Institute*

Many electron correlated scattering

POSTER 3
5:00PM-7:00PM

1 - Sungwan Choi *Korea Advanced Institute of Science and Technology*
Modification of Lanczos method for high fidelity and scalability for electronic structure calculations

2 - Thomas Collins *Oklahoma State University*
A framework for causal, quantum biology consistent with thermodynamics

3 - Ana Paula de Lima Batista *Universidade de Sao Paulo*
New derived-N-heterocyclic olefins compounds for CO_2 capture: a computational study

4 - Brendon Disrud *North Dakota State University*
Molecular dynamics of reactions between hydrogen peroxide and zigzag carbon nanotube

5 - Shuichi Fukuyoshi *Kanazawa University*
Evaluations of density functionals and solvation effect for racemization reaction of amino acid residues

6 - Min Gao *Hokkaido Unviersity*
Promising catalytic activity of h-BN monolayer by doping C atoms

7 - Jie Gu *University of Florida*
Adiabatic spin pump through an antiferromagnetic molecular magnet

8 - Hirotaka Kitoh-Nishioka *Center for Computational Sciences, University of Tsukuba*
Singlet fission couplings calculated with complete-active-space self-consistent field (CASSCF) theory

9 - Devin Matthews *The University of Texas at Austin*
Keeping quantum chemistry simple: two tales

10 - Vincent Ortiz *Auburn University*
Electron propagator theory and correlation-bound anions

11 - Takat Rawal *University of Central Florida*
Computational design of MoS_2-based catalysts for methanol synthesis from syngas

12 - Varun K. Rishi *University of Florida*
The reach and limits of a 'double excitations only' model in coupled cluster theory

13 - Francisca Sagredo *University of California, Irvine*
Investigating ensemble density functional theory on the Hubbard model

14 - Wendi Sapp *University of South Dakota*
Enhancing detection with DFT and MBPT: charge mobility in a Germanium dark matter detector

15 - Braden Weight *North Dakota State University*
Non-covalent functionalization of carbon nanotubes: controlling chirality selectivity via alkyl groups of conjugated co-polymers

POSTER 4
9:00PM-11:00PM

1 - Antonio Cancio *Ball State University*

Fitting a round peg into a round hole - a generalized gradient approximation based upon the asympototic analysis of atomic correlation energies

2 - Eduardo Chamorro *Universidad Andres Bello*

Applications of the intrinsic electrophilicity and nucleophilicity indices

3 - Antonio G. S. De Oliveira-Filho *Universidade De Sao Paulo*

Coupled cluster, density functional theory or experiment? A benchmark study of diatomic molecules containing transition metals

4 - Frank Hagelberg *East Tennessee State University*

Spin filter properties of armchair graphene nanoribbons with substitutional Fe atoms

5 - Dmitri Kilin *North Dakota State University*

N2: non-collinear spin with nonadiabatic dynamics for lanthanide spectroscopy: from photoinduced dynamics to photoluminescence

6 - Svetlana Kilina *North Dakota State University*

Modeling of relaxation and decoherence processes at the interfaces of ligated and core/shell quantum dots

7 - Shuanglong Liu *University of Florida*

A two-dimensional organometallic field effect transistor with gaint magnetoresistance

8 - Adrian Morrison *The Ohio State University*

Evidence for a vibronic singlet fission mechanism from ab initio non-adiabatic coupling calculations of crystalline tetracene

9 - Jonathan Moussa *Sandia National Laboratories*

Localized and randomized linear-scaling algorithms for electronic structure

10 - Whitney Ong *North Dakota State University*

Oxidation of PbSe quantum dots: insights from first-principle calculations

11 - Muhammad Shahbaz *University of Delaware*

Dispersion energy in density-functional theory

12 - Yongxin Yao *Ames Laboratory - US DOE*

Benchmark calculations of the correlation matrix renormalization method for a molecule test set

13 - Yue Yu *University of Florida*

Hydrogen release exploration and mobility calculation

14 - Long Zhang *University of Florida*

DFT+DMFT study of monolayer MoS2

Wednesday, February 22, 2017

Plenary 4 - Density Functional Theory Including van der Waals Forces
8:30am-9:50am

Chair: Dieter Cremer *Southern Methodist University*

Timo Thonhauser *Wake Forest University*

Capturing van der Waals interactions in DFT through non-local exchange and correlation

Alexander Tkatchenko *University of Luxembourg*

Many-body dispersion interactions: the tail that wags the dog

Gerit Brandenburg *University College London*

Density functional theory including van der Waals forces

Invited 4 - Many-Electron Theory of Molecular Interactions
10:15am-11:45am

Chair: Elfi Kraka *Southern Methodist University*

Maria Pilar de Lara-Castells *Institute of Fundamental Physics*

Modeling of the soft, ^{4}He droplet-mediated, deposition of metallic nanoparticles: an intermolecular interaction problem

Krzysztof Szalewicz *University of Delaware*

Dispersion energy

Jordan R Schmidt *UW Madison*

Recent advances in first-principles force-field development using SAPT: approaching quantitative accuracy with transferable site-site potentials

Ilya Kaplan *Instituto De Investigaciones en Materiales, UNAM*

Symmetry properties of the electron density and following from it limits on the DFT applications

Selected Hot-Topic Talks 3
1:30pm-3:00pm

Chair: Paul Seybold *Wright State University*

Elvira Sayfutyarova *Princeton University*

Building active spaces automatically and systematically from atomic valence orbitals

Ulises Miranda *Semenov Institute of Chemical Physics, RAS*

Structure of the In_2O_3 molecule in the free state and in the crystal

Andrew Mahler *Texas Christian University*

When LDA provides the highest reaction barriers: insight into quantum chemistry from density functional theory

Hemanadhan Myneni *University of Delaware*

Theoretical studies on the effect of strong magnetic fields on the interaction energies of water

Eugene DePrince *Florida State University*

Variational optimization of the two-electron reduced-density matrix under pure-state N-representability conditions

Wednesday, February 22, 2017

Selected Hot-Topic Talks 3 - Continued
1:30pm-3:00pm

Chair: Paul Seybold *Wright State University*

José Luis Gázquez *Universidad Autónoma Metropolitana-Iztapalapa*
Analysis of GGA exchange energy functionals with correct asymptotic behavior of the corresponding potential

Luis Rincon *Universidad San Francisco de Quito*
The electron localization as the information gain of the conditional pair density

Robert Topper *Cooper Union for the Advancement of Science & Art*
Unusual hydrogen bond diversity in ammonium halide nanoclusters

Dane Hogoboom *North Dakota State University*
A compuutational study of dimethyl-hydrazine combustion

Markus Eisenbach *Oak Ridge National Laboratory*
Fully relativistic ab initio calculations using multiple scattering theory for non-spherical space filling potentials

Jorge Seminario *Texas A&M University*
Simulations of the first charge of nanobatteries: silicon anodes

Poster 5
9:00pm-11:00pm

1 - Andrew Brooks *University of Florida*
Modeling anomalous hysteresis in hybrid perovskite with space charge limited currents

2 - Eike Caldeweyher *University of Bonn*
Development and implementation of D4: A charge dependent molecular dispersion coefficient model

3 - Aaron Forde *North Dakota State University*
Morphology influence on hole transfer - spatial locality versus explicit ligand coordination: case study of dye-sensitized lead halide perovskite solar cells

4 - Yulun Han *North Dakota State University*
Photofragmentation of tetranitromethane: spin-unrestricted time-dependent excited-state molecular dynamics

5 - Toshiyuki Hirano *The University of Tokyo*
A theoretical study of glucose oxidase using canonical molecular orbital calculation

6 - Mohammed A. Jabed *North Dakota State University*
Structural photophysical properties of cytosine and guanine ligated Ag cluster

7 - Kazutomo Kawaguchi *Kanazawa University*
Theoretical study of a coarse grained model of electrostatic interaction between protein molecules

8 - Run Li *University of North Dakota*
Parallelization of triple and quadruple perturbation corrections to multireference CISD

Wednesday, February 22, 2017

Poster 5 - Continued
9:00pm-11:00pm

9 - Levi Lystrom *North Dakota State University*
DFT insights into mechanisms of brightening of CdSe quantum dots by hydrides

10 - Yu-Ya Ohnishi *Kobe University*
Explicitly correlated second-order Green's function (GF2-F12) for ionization energies

11 - Bo Peng *Pacific Northwest National Laboratory*
Low-rank factorization of electron integral tensors and its application in electronic structure theory

12 - William Perry *University of Florida*
A method for fast approximation of the phonon density of states in crystals

13 - Karnamohit Ranka *University of Florida*
Reaction profile and chemical kinetics study of [$C(^1D/^3P) + SiH_4$]

14 - Bidhan Saha *Florida A&M University*
Elastic collisions of electrons and positrons by Na atoms

15 - Daisuke Yamaki *Research Organization for Information Science and Technology (RIST)*
Difference density matrix analysis of epigenetic chemical modifications

Thursday, February 23, 2017

Plenary 5 - Quantum Materials and Spectroscopy
8:30am-10:30am

Chair: Noa Marom *Carnegie Mellon University*

Thomas Maier *Oak Ridge National Laboratory*
New developments in dynamical cluster quantum Monte Carlo theory

Thomas Devereaux *Stanford University and SLAC*
Fluctuating stripes in 3-band Hubbard models from DMRG and DQMC simulations

Warren Pickett *UC Davis*
Topological quantum materials: designed Chern insulators, natural nodal loop semimetals

Thursday, February 23, 2017

Plenary 6 - Complex and Functional Materials
10:50am-12:50pm

Chair: Xiaoguang Zhang *University of Florida*

Lin-Wang Wang *Lawrence Berkeley National Laboratory*

Carrier localizations due to nanoscale pattern, ordering and random fluctuations

Janice Musfeldt *University of Tennessee*

Magnetoelectric coupling across the spin flop transition in Ni_3TeO_6

De-En Jiang *University of California, Riverside*

Understanding functional materials for catalysis

Plenary 7 - Machine Learning and Algorithms
2:00pm-4:00pm

Chair: Sam Trickey *University of Florida*

Kieron Burke *University of California, Irvine*

Machine learning density functionals

Aldo Romero *West Virginia University*

From metaheuristic to dynamical crystal structural search from first principles

John Herbert *The Ohio State University*

First-principles exciton models

Plenary 8 - Synthesis and High Throughput
4:15pm-6:15pm

Chair: Jim Greer *Tyndall National Institute*

Shyue Ping Ong *University of California, San Diego*

Creating it from bit: designing materials by integrating quantum mechanics, informatics and computer science

Hai-Ping Cheng *University of Florida*

Understanding the role of f-electrons in Mn^{III}-Ce^{IV}-Mn^{III}

Friday, February 24, 2017

Plenary 9 - Core Excitation Spectroscopy
8:30am-10:30am

Chair: John Stanton *University of Florida*

Nick Besley *University of Nottingham*

Simulation of X-ray absorption and X-ray emission spectroscopy

Lan Cheng *Johns Hopkins University*

Scalar relativistic equation-of-motion coupled cluster calculations of core ionized/excited states

Sonia Coriani *DTU Chemistry - Technical University of Denmark*

Coupled cluster strategies for core spectroscopies of ground and excited states

Invited 5 - Fifty Year Anniversary of Jiří Čižek Paper
10:50am-12:50pm

Chair: Rodney Bartlett *University of Florida*

Josef Paldus *University of Waterloo*

Early days of CC theory and a glimpse in the future

Piotr Piecuch *Michigan State University*

The 1966 Journal of Chemical Physics article by Jiří Čížek: what is in it and why is it so important

Miroslav Urban *Comenius University*

From early days of the coupled cluster theory to its role as a predictive and benchmark instrument in computational chemistry

John Stanton *University of Florida*

Coupled-cluster theory and Born-Oppenheimer breakdown

Jozef Noga *Comenius University in Bratislava*

Pair coupled cluster doubles F12 approach

INVITED 6 - COUPLED-CLUSTER THEORY AND THE FUTURE
2:30PM-6:25PM

Chair: Ajith Perera *University of Florida*

Henry Schaefer *University of Georgia*

Density cumulant functional theory: benchmarks and applications

Mihály Kállay *Budapest University of Technology and Economics*

Reduced-cost linear-response CC2 method based on natural orbitals and natural auxiliary functions

Krzysztof Szalewicz *University of Delaware*

Coupled cluster method with explicitly correlated gaussian functions

Karol Kowalski *Pacific Northwest National Laboratory*

Universal state-selective approach to multi-reference coupled-cluster theory

Daniel Kats *University of Stuttgart*

Linear scaling multireference coupled cluster methods

Steven Gwaltney *Mississippi State University*

Reduced active spaces and external correlation

Monika Musial *University of Silesia in Katowice*

Fock space multireference coupled cluster method in the studies of the electronic structure of atoms and molecules

Sourav Pal *Indian Institute of Technology Bombay*

Coupled-cluster theories including relativistic effects and complex absorbing potential for unbound states

Dmitry Lyakh *Oak Ridge National Laboratory*

Efficient electronic structure theory via scale-adaptive coupled-cluster formalism

Peter Szalay *Eötvös Loránd University, Institute of Chemistry*

Investigation of the impact of different terms in the second order Hamiltonian on excitation energies of valence and Rydberg states

So Hirata *University of Illinois at Urbana-Champaign*

New frontiers of coupled-cluster theory: solid-state applications, anharmonic vibrational analog, finite-temperature extension, explicit correlation, automated implementation, and general-order algorithm

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Notes

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POSTER 1 Monday February 20 5:15 PM - 7:00 PM	POSTER 3 Tuesday February 21 5:15 PM - 7:00 PM	POSTER 5 Wednesday February 22 5:15 PM - 7:00 PM
1. Alex Bazante 2. Joanna Bednarska 3. Daniel Chaves Claudino 4. Jun Jiang 5. Yifan Jin 6. Ryo Kiribayashi 7. Lukas Konecny 8. Shubin Liu 9. Johannes Margraf 10. Yuki Mitsuta 11. Satoshi Nakagawa 12. Youngchoon Park 13. Duminda Ranasinghe 14. Paul G. Seybold 15. D. Jonathan Vogel	1. Sungwan Choi 2. Thomas Collins 3. Ana Paula de Lima Batista 4. Brendon Disrud 5. Shuichi Fukuyoshi 6. Min Gao 7. Jie Gu 8. Hirotaka Kitoh-Nishioka 9. Devin Matthews 10. Vincent Ortiz 11. Takat Rawal 12. Varun K. Rishi 13. Francisca Sagredo 14. Wendi Sapp 15. Braden Weight	1. Andrew Brooks 2. Eike Caldeweyher 3. Aaron Forde 4. Yulun Han 5. Toshiyuki Hirano 6. Mohammed A. Jabed 7. Kazutomo Kawaguchi 8. Run Li 9. Levi Lystrom 10. Yu-Ya Ohnishi 11. Bo Peng 12. William Perry 13. Karnamohit Ranka 14. Bidhan Saha 15. Daisuke Yamaki

POSTER 2 Monday February 20 9:00 PM - 11:00 PM	POSTER 4 Tuesday February 21 9:00 PM - 11:00 PM
1. Marta Choluj 2. Marc Coons 3. Adam Erck 4. Takeshi Iwasa 5. Muneaki Kamiya 6. Megumi Kayanuma 7. Elvis Maradzike 8. Michael Metz 9. David Micha 10. Wayne Mullinax 11. Tomoki Nakayoshi 12. Daniel Nascimento 13. Tetsuya Taketsugu 14. Kizashi Yamaguchi	1. Antonio Cancio 2. Eduardo Chamorro 3. Antonio G. S. De Oliveira-Filho 4. Frank Hagelberg 5. Dmitri Kilin 6. Svetlana Kilina 7. Shuanglong Liu 8. Adrian Morrison 9. Jonathan Moussa 10. Whitney Ong 11. Muhammad Shahbaz 12. Yongxin Yao 13. Yue Yu 14. Long Zhang