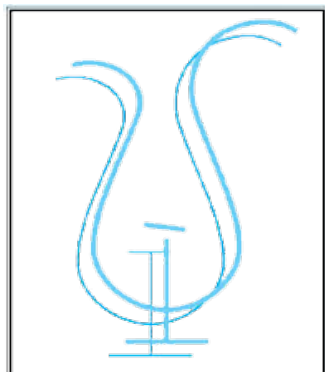


59TH SANIBEL SYMPOSIUM



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FEBRUARY 17-22, 2019

THE KING AND PRINCE, ST. SIMONS ISLAND, GA, USA

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PROGRAM

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

Sunday, February 17	9
Plenary 1 - A Celebration of the Science of Klaus Ruedenberg	9
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Reception	
Delegal Room 9:00pm-11:00pm	
<i>Two complimentary drink tickets will be provided</i>	
Monday, February 18	9-13
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Plenary 5 - Relativistic Quantum Mechanics	20
Plenary 6 - Search for Novel Magnetic Systems	20
Plenary 7 - Big Data and Machine Learning	20
Plenary 8 - Quantum Computing	21
Symposium Banquet Cocktails, Hotel Lawn (weather permitting) 7:00pm-8:00pm <i>One complimentary drink ticket will be provided</i> Dinner, Delegal Room 8:00pm-11:00pm Post-Banquet Speaker - Mark Gordon	
 Friday, February 22	 21
Plenary 9 - Theory and Methods for Thermoelectrics	21
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WELCOME

Klaus Ruedenberg is a giant in electronic structure theory. An early 1955 explanation of much of the electronic spectra for pi-electron systems originated with free-electron molecules in the hands of Ruedenberg. From there, his work was the first to introduce general localized orbitals, present even-tempered Gaussian basis sets, and define the FORS model (Fully Optimized Reaction Space) as a systematic approach to doing complete active-space, multi-configuration interaction calculations. During his very extensive career, perhaps the most common element has been his work on understanding the “nature of the chemical bond.” The 59th Sanibel meeting will specifically address these fundamental developments, and some new ones, as it celebrates the science and career of Klaus Ruedenberg.

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-five 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 59TH SANIBEL SYMPOSIUM IS SPONSORED BY:

Ames Laboratory
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AWARDS:

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PROCEEDINGS PUBLISHER:

Taylor and Francis

GENERAL INFORMATION

Dates

Sunday, February 17 - Friday, February 22, 2019

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, the Sunday Reception, morning and afternoon beverage breaks, and the Banquet Dinner on Thursday night. All other meals are on your own. A one-day registration does not include the Thursday Banquet.

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

Sunday, February 17th: 12:00pm-7:00pm
Monday, February 18th: 8:00am-5:00pm
Tuesday, February 19th: 8:00am-5:00pm
Wednesday, February 20th: 8:00am-5:00pm
Thursday, February 21st: 8:00am-5:30pm
Friday, February 22nd: 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 causes an undue burden on the Session Chair and ultimately deprives subsequent speakers of their rightful allotted 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 (full week only) and are also open to registrants' guests for whom a banquet ticket has been purchased. There are two scheduled social events:

Sunday Evening - Opening Reception

9:00pm to 11:00pm - The Opening Reception, generously sponsored by Iowa State University and the Ames Laboratory, will take place in the Delegal Room. Join us for light hors d'oeuvres, desserts, and two 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

7:00pm to 8:00pm - One complimentary drink 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.

8:00pm to 11:00pm - Dinner will be served in the Delegal Room. In addition to the banquet dinner, there will be a post-dinner speaker, Mark Gordon, and presentation of awards. To indicate your choice of menu, please display your colored meal preference coupon.

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

Speaker Instructions

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

- 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.

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 59th Sanibel Symposium.

Abstract Access

All abstracts for the 59th 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. 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 2019 Sanibel Symposium are eligible to be submitted to the proceedings issue of Molecular Physics. To ensure rapid publication of the proceedings, contributors must submit completed manuscripts to Molecular Physics electronically. Submission must be completed by April 30, 2019. The instructions for submissions can be found at <http://mc.manuscriptcentral.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 2019 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

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Erik Deumens
Frank E. Harris
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Hendrik Monkhorst
N. Yngve Öhrn
Ajith Perera
Simon Phillpot
John R. Sabin
Beverly A. Sanders
John F. Stanton
Samuel B. Trickey
Xiaoguang Zhang

External Organizer:

Mark Gordon
Iowa State University

Symposium Coordinator:

Galyna Vakulenko

Audio, Video, and IT:

Clint Collins

Proceedings Editor:

Rodney J. Bartlett

Sanibel Symposium Endowment

The longevity of the Sanibel Symposium's engagement of international scientists in atomic, molecular, biomolecular, 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 10,000 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 Hotel 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 Sanibel 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 buildings or 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 such pursuits. Therefore, we appeal to you 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, Sanibel Organizer
University of Florida
Quantum Theory Project
P.O. Box 118435
Gainesville, FL 32611



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



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 SUNDAY, FEBRUARY 17, 2019 

PLENARY 1 - A CELEBRATION OF THE SCIENCE OF KLAUS RUEDENBERG
2:00PM-4:45PM

Chair: Henry F. Schaefer

University of Georgia

Sharon Hammes-Schiffer

Yale University

Multicomponent quantum chemistry: integrating electronic and nuclear quantum effects

Sotiris Xantheas

Pacific Northwest National Laboratory

The many-body expansion for aqueous systems revisited

Thom Dunning

University of Washington

Models and methods in theoretical & computational chemistry

INVITED 1 - A CELEBRATION OF THE SCIENCE OF KLAUS RUEDENBERG
5:00PM-6:45PM

Chair: Michael Schmidt

Iowa State University

Lyudmila Slipchenko

Purdue University

Polarizable embedding for biological systems: Modeling photoactive proteins with the effective fragment potential method

Gernot Frenking

Philipps-University of Marburg

Travelling in valence space

Klaus Ruedenberg

Iowa State University

Covalent chemical binding

 MONDAY, FEBRUARY 18, 2019 

PLENARY 2 - NON-ADIABATIC DYNAMICS
8:30AM-10:30AM

Chair: Dmitri Kilin

North Dakota State University

William Miller

University of California, Berkeley

Classical molecular dynamics simulations of electronically non-adiabatic processes

Joseph Subotnik

University of Pennsylvania

Edminston-Ruedenberg diabatic states, nonadiabatic dynamics and magnetic fields

Victor Batista

Yale University

Tensor train algorithms for quantum dynamics simulations of excited state nonadiabatic processes and quantum control

≡ MONDAY, FEBRUARY 18, 2019 ≡

INVITED 2 - NOVEL THEORY AND APPLICATIONS

10:50AM-12:50PM

Chair: Monika Musial

University of Silesia in Katowice

Laura Gagliardi

University of Minnesota

Multireference methods for molecular and periodic systems

Bernard Kirtman

University of California, Santa Barbara

Electronic orbital response of infinite periodic systems to uniform external magnetic fields

Douglas Klein

Texas A&M University

Non-bonding unpaired electrons in decorated graphene

David Tew

Max Planck Institute for Solid State Research

Quasi-robust local density fitting

SELECTED HOT-TOPIC TALKS 1

2:30PM-5:45PM

Chair: Jane Murray

University of New Orleans

Varun Rishi

Virginia Tech

Treating strong correlation with internally corrected coupled cluster methods: Is the distinguishable cluster approach systematically improvable?

Punit Jha

University of Illinois at Urbana-Champaign

Numerical evidence invalidating finite-temperature many-body perturbation theory

Mark Iron

Weizmann Institute of Science

Density functional theory and transition metals reactions – Navigating the alphabet soup of functionals

Yixuan Wang

Albany State University

Exploring the binding mechanism of inverse agonists against estrogen-related receptor alpha with multiscale molecular modeling

Joachim Sauer

Humboldt-Universität zu Berlin

Ab initio calculations with chemical accuracy for molecule-surface interactions

James Thorpe

University of Florida

Dangers of the SCF-level DBOC: NO and NO₄ as examples

Steven Valone

Pennsylvania State University

Model “hybrid+U” density functional from constrained search combined with wave function theory

António Varandas

University of Coimbra

From optimal basis sets to accurate potentials: Elemental carbon clusters at the focal point

Isuru Ariyarantha

Auburn University

Aufbau rules for solvated electron precursors: The case of Be(NH₃)₄₀[±]

Joshua Black

University of Stuttgart

Linear and quadratic internally contracted multireference couple-cluster approximations

Valentin Karasiev

University of Rochester

Exchange-correlation thermal effects: Softening the deuterium Hugoniot and thermophysical properties

POSTER 1
7:45PM-9:00PM

Isuru Ariyaratna

Auburn University

Molecules mimicking atoms: Monomers and dimers of $\text{Li}(\text{NH}_3)_4$ and $\text{Na}(\text{NH}_3)_4$

Dmytro Bykov

Oak Ridge National Laboratory

Multilayer divide-expand-consolidate linear-scaling coupled cluster methods

Kade Head-Marsden

University of Chicago

Non-Markovian dynamics: An extension of the Lindblad theory

Landon Johnson

North Dakota State University

Modeling charge carrier dynamics at perovskite/charge transport material interface using density functional theory and Redfield theory

Dmitry Liakh

Oak Ridge National Laboratory

ExaTN: C++ numerical primitives for tensor network HPC simulations in quantum many-body theory

Joani Mato

Iowa State University

Examining the ground- and excited-state potential energy surfaces with spin-flip ORMAS: Minima, saddle points and conical intersections

Nelanie Mora-Díez

Thompson Rivers University

Theoretical study of deuterium isotope effects on acidity at ambient and hydrothermal conditions

Tomoki Nakayoshi

Meijo University

Computational studies on pyroglutamylation mechanism of N-terminal glutamic acid residues in aqueous conditions

Thanh Lam Nguyen

University of Florida

Three-dimensional master equation (3DME) approach

Youngchoon Park

University of Florida

Core excitation spectra from the time-dependent approach of the coupled-cluster and density functional theory

Buu Pham

Iowa State University

Compressing the four-index two-electron repulsion integral matrix using the resolution-of-the-identity approximation combined with the proper rank factorization approximation

Luis Rincon

Universidad San Francisco de Quito

How good is DFT for no-pairs ferromagnetic bonds?

Benjamin Rudsteyn

Columbia University

Accurate quantum chemistry of organic molecules and metal complexes with auxiliary-field quantum Monte Carlo

Tosaporn Sattasathuchana

Iowa State University

An accurate and efficient development of QM/EFP: Parallelization

Michael Schmidt

Iowa State University

Valence virtual orbitals

Anatoly Stepanov

Belorussian State University

Information entropy of molecular structure modification

Naoki Tanabe

Hiroshima City University

Molecular dynamics study of structural fluctuations in CDR-H3 of anti-HIV antibodies PG9 and PG16

Pawel Tecmer

Nicolaus Copernicus University

Quantum chemical description of excitation energies in heavy elements

POSTER 2
9:10PM-10:30PM

- Gustavo Aucar** *Northeastern University of Argentina*
Magnetic interactions in small fragments of DNA base pairs
- Samraghi Banerjee** *Ohio State University*
Dynamical algebraic diagrammatic construction approach for X-ray photoelectron spectra
- Megan Bentley** *University of Florida*
The adiabatic ionization energy of the vinoxy radical
- Denis Bokhan** *University of Florida*
Spin-orbit splitted excited states using explicitly-correlated equation-of-motion coupled cluster singles and doubles eigenvector
- Prateek Goel** *University of Florida*
The adventures of Siegert eigenvalues
- Yulun Han** *North Dakota State University*
First principles study on grafting of diazonium salts to silicon surfaces
- Josh Hinz** *University of Rochester*
Deorbitalized meta-GGA with the long range van der Waals exchange-correlation functional calculations of the insulator-metal transition of hydrogen
- Kohey Ishikawa** *University of Tsukuba*
Effects of hinge-loop mutation on electron transfer rate between two heme groups in Cytochrome c heterodimer
- Ernesto Martinez Baez** *Washington State University*
Al-alkali ion-pairing interactions and its influence in the ^{27}Al NMR shielding tensor from AIMD ensemble averaging standpoint
- Shubham Pandey** *University of Florida*
Sequestration of radionuclides in metal-organic frameworks from first principles calculations
- Reetam Paul** *University of Rochester*
High-pressure phases and spectral properties of silicon
- Ruojing Peng** *Ohio State University*
Simulating X-ray absorption spectra with density cumulant theory
- Alberto Perez** *University of Florida*
Sampling low free energy protein structures in high dimensional conformational landscapes
- Daniel Ramirez** *North Dakota State University*
Excited state dynamics in 2D perovskite thin films: Roles of surface ligands
- Toru Saito** *Hiroshima City University*
Quantitative assessment of reparameterized PM6 (rPM6) for hydrogen atom transfer reactions
- Aleksander Wysocki** *Virginia Tech*
Magnetic properties of TbPc_2 -type single-molecule magnets from first principles quantum-chemical calculations
- Stephen Xie** *University of Florida*
Machine learning of potential-energy landscapes with support-vector machines and neural networks

≡ MONDAY, FEBRUARY 18, 2019 ≡

POSTER 2 - CONTINUED

9:10PM-10:30PM

Peng Xu

Iowa State University

New implementation of QM/EFP2: A benchmarking study on S22 and S66 data sets

≡ TUESDAY, FEBRUARY 19, 2019 ≡

PLENARY 3 - QUANTUM CHEMISTRY AND THE ENVIRONMENT

8:30AM-10:30AM

Chair: Devin Matthews

Southern Methodist University

Joseph Francisco

University of Pennsylvania

Water effects on atmospheric reactions

Aurora Clark

Washington State University

When chemical intuition fails: The importance of hierarchical chemical environments when studying environmental problems

Vassiliki Glezakou

Pacific Northwest National Laboratory

A dynamic picture of chemical bonding and entropic effects from large scale molecular simulations

INVITED 3 - CHEMICAL BONDS, THEN AND NOW

10:50AM-12:50PM

Chair: Svetlana Kilina

North Dakota State University

Mark Pederson

U.S. Department of Energy

Use of Edmiston-Ruedenberg and Fermi-Löwdin orbitals in orbital-based quantum theories

Frank Weinhold

University of Wisconsin-Madison

Resonance theory reboot

Manual Yáñez

Universidad Autónoma de Madrid

Bonding perturbations triggered by intrinsically electron-deficient systems

Joseph Ivanic

Frederick National Laboratory for Cancer Research

A novel hybrid correlation energy (HyCE) approach based on separate evaluations of internal and external components

SELECTED HOT-TOPIC TALKS 2
2:30PM-5:45PM

Chair: J. Vincent Ortiz	Auburn University
Timo Thonhauser <i>Van der Waals density functional with corrected long-range behavior</i>	Wake Forest University
Fabian Faulstich <i>Numerical and theoretical aspects of the DMRG-TCC method exemplified by the nitrogen dimer</i>	University of Oslo
Aliaksei Mazheika <i>Discovering better catalysts from artificial intelligence analysis of ab initio data: Application to the CO₂ conversion problem</i>	Fritz-Haber-Institute of the Max-Planck-Society
Pavel Pokhilko <i>A new implementation of spin-orbit couplings for EOM-CC and their analysis</i>	University of Southern California
Gregory Tschumper <i>Halide ion hydration: Big challenges from small ions</i>	University of Mississippi
Yifan Jin <i>Correlation-consistent composite approach based on distinguishable cluster approximation</i>	Michigan State University
Alexandra Raeber <i>Current-constrained reduced density-matrix theory for molecular conductivity</i>	University of Chicago
José Gazquez <i>Exchange energy functional in the generalized gradient approximation with nearly correct asymptotic potential</i>	Universidad Autonoma Metropolitana-Iztapalapa
Avijit Shee <i>Exploration of coupled cluster Green's function in the framework of self-energy embedding theory (SEET)</i>	University of Michigan
Roland Lindh <i>Ab initio calculation on muonic atoms and molecules</i>	Uppsala University
Claudia Viquez <i>QM/EFP excitations: Is polarizable embedding good enough?</i>	Purdue University
Ari Chakraborty <i>Efficient calculation of excitation energies using locally-projected real-space geminal electron-hole interaction kernel</i>	Syracuse University

POSTER 3
7:45PM-9:00PM

Gustavo Aucar <i>Microsolvation and solvent effects on NMR magnetic shieldings of solvated I⁻ anion</i>	Universidad Nacional del Nordeste
Fatima Benyettou <i>Quantum chemistry study of water ab initio calculation</i>	University of Mohamed Boudiaf

POSTER 3 - CONTINUED
7:45PM-9:00PM

- Sebastian Ehlert** *University of Bonn*
A generally applicable atomic-charge dependent London dispersion correction scheme
- Anastasia Gunina** *Iowa State University*
Hybrid OpenMP/MPI implementation of the EFMO method in GAMESS
- Sarah Johnson** *University of Mississippi*
Probing non-covalent interactions driving molecular assembly in organo-electronic building blocks
- Svetlana Kilina** *North Dakota State University*
Effect of electron induction abilities of functional groups on lowest excitons in covalently functionalized C
- Hiroataka Kitoh-Nishioka** *University of Tsubaka*
Fragment molecular orbital study on electron tunneling in protein
- Venkata Kolluru** *University of Florida*
Implicit self-consistent description of electrolyte in plane-wave density-functional theory
- Maricris Mayes** *University of Massachusetts Dartmouth*
Noncovalent interactions in tyrosine-based dipeptide dimers
- Nelanie Mora-Díez** *Thompson Rivers University*
Macroscopic pKa prediction of polyprotic acids from DFT calculations: The case of acetohydroxamic acid
- Monika Musiał** *University of Silesia in Katowice*
The coupled cluster theory generalized for the description of the high spin ionized states via equation-of-motion philosophy
- Vincent Ortiz** *Auburn University*
Electron-propagator calculations with generalized Hartree-Fock spin-orbitals
- Morgan Perkins** *University of Mississippi*
Conformational analysis of semiconducting organic oligomers
- Moneesha Ravi** *University of Florida*
Approximate spin-adapted treatment of single reference coupled cluster for open-shell molecules
- Thomas Sexton** *University of Mississippi*
Structures, energetics and harmonic vibrational frequencies of hydrated halide ions by the 2-body:many-body method
- Masafumi Tsuyuki** *Keio University*
Graphical and cDFT approaches to the study of fundamental and overtone absorption intensities of some OH stretching vibrations
- Roderick Wasylishen** *University of Alberta*
Isotope effects on magnetic resonance parameters in hydrogen bonded systems

POSTER 4
9:10PM-10:30PM

- Katharina Boguslawski** *Nicolaus Copernicus University*
Inexpensive electron-pair methods to model ground and excited states across the periodic table
- Antonio Cancio** *Ball State University*
Asymptotic analysis of atomic Pauli potentials
- Carlos Diaz** *University of Texas El Paso*
Scalability improvements to NRLMOL for DFT calculations of large molecules
- Fatima Fatima** *North Dakota State University*
Lifetimes of photoinduced hot charge carriers influenced by momentum dispersion in silicon nanowires
- Aaron Forde** *North Dakota State University*
Computational study of polaron emission in a lead-halide perovskite nanocrystal
- Toshiuki Hirano** *University of Tokyo*
GPU acceleration of a canonical molecular orbital calculation program by the third-generation density-functional-theory-based method
- Der-you Kao** *NASA Goddard Space Flight Center*
Impact of self-interaction correction on the electronic and magnetic structures of a tri-anionic molecule
- Elvis Maradzike** *Florida State University*
A dynamical correlation model for variational two-electron reduced density matrix driven complete active space self-consistent field methods
- David Micha** *University of Florida*
Atomistic treatments of electronic relaxation at photoexcited semiconductor surfaces
- Joshua Paul** *University of Florida*
Discovery and characterization of 1D materials via data mining and DFT
- James Shee** *Columbia University*
Predictions of transition metal thermochemistry and singlet-triplet gaps for organic diradicals via quantum Monte Carlo
- Ron Shepard** *Argonne National Laboratory*
On the mean energy state average condition
- Linyuan Shi** *University of Florida*
Carbon fiber oxidation under high temperature by ReaxFF based molecular dynamics simulation
- Dmitry Skachkov** *University of Florida*
Magnetic state of single-molecule magnetic complex $[\text{Mn}_{12}\text{O}_{12}(\text{O}_2\text{CH})_{16}(\text{H}_2\text{O})_4]$
- Anne Marie Tan** *University of Florida*
First-principles investigation of charged point defects in MoS_2
- Libor Veis** *University of Florida*
Coupled cluster methods tailored by matrix product state wave functions

≡ TUESDAY, FEBRUARY 19, 2019 ≡

POSTER 4 - CONTINUED
9:10PM-10:30PM

Zachary Windom

University of Florida

Ab initio molecular dynamics simulations to understand speciation and solvation structure of the glyphosate herbicide

Yoh Yamamoto

University of Texas at El Paso

Performance of metaGGA functional using the self-interaction corrected density from the Fermi-Lowdin orbital self-interaction correction method

≡ WEDNESDAY, FEBRUARY 20, 2019 ≡

PLENARY 4 - DENSITY FUNCTIONAL THEORY
8:30AM-10:30AM

Chair: Valentin Karasiev

University of Rochester

Neepa Maitra

Hunter College

Going beyond the adiabatic approximation in TDDFT

Nikitas Gidopoulos

Durham University

Optimal power series expansions of the Kohn-Sham potential

Hannes Jónsson

University of Iceland

Self-interaction corrected energy functional applied to molecules and solids

INVITED 4 - ACCURATE QUANTUM CHEMISTRY
10:50AM-12:50PM

Chair: Vassiliki Glezakou

Pacific Northwest National Laboratory

Hans Jørgen Jensen

University of Southern Denmark

Status and perspectives for the multiconfigurational short-range density functional theory method

Eric Neuscamman

University of California, Berkeley

New opportunities in excited state quantum chemistry

Sourav Pal

Indian Institute of Science Education and Research

Complex absorbing potential based coupled cluster theory for autoionizing states

Klaus Ruedenberg

Iowa State University

Quantum chemistry, now and then

SELECTED HOT-TOPIC TALKS 3
2:30PM-5:45PM

Chair: Ron Shepard	Argonne National Laboratory
Richard Lyngdoh <i>Metal-metal bond distances and bond orders for binuclear complexes of 3D-block Metals Ti through Zn: Theory and experiment compared</i>	North-Eastern Hill University
William Perry <i>Ligand optimization for the spin-lattice coupling of single-molecule magnets Mn_3</i>	University of Florida
Yue Yu <i>First-principles resonant Raman spectroscopy for 2D materials</i>	University of Florida
Xiaoyan Cao <i>Relativistic effects in photoluminescence and photocatalysis of transition metal systems</i>	University of Cologne
Lan Cheng <i>Two-component spin-orbit coupled cluster methods using mean-field spin-orbit integrals</i>	Johns Hopkins University
Lukas Pasteka <i>Material size dependence on fundamental constants</i>	Comenius University
Noor Khan <i>Theoretical study of a complete catalytic cycle for methane to methanol transformation facilitated by metal methoxides</i>	Auburn University
Johannes Margraf <i>Exchange-correlation energy density from coupled cluster theory</i>	Technical University of Munich
Minh Nguyen <i>Aromaticity: A never-ending story</i>	Katholieke Universiteit Leuven
Hao Li <i>Quantum interferometry using entangled photons</i>	University of Houston
Alberto Vela <i>A comparative DFT and CCSD study of spin-crossover in mononuclear transition metal complexes</i>	CINVESTAV
Andre Laestadius <i>Monotonicity in coupled cluster methods</i>	University of Oslo

POSTER 5
7:45PM-9:00PM

Ashleigh Barnes <i>Massively parallel and GPU-accelerated implementation of the third-order cluster perturbation method for excitation energy calculations</i>	Oak Ridge National Laboratory
Jiri Brabec <i>Massively parallel DMRG code for quantum chemistry</i>	Czech Academy of Sciences

POSTER 5 - CONTINUED
7:45PM-9:00PM

- Andrew Brooks** *University of Florida*
Temperature-dependent carrier mobility in methylammonium lead iodide
- Dianteng Chen** *University of Florida*
Calculation of exchange coupling constants in Mn-Ce molecular magnets
- Jie Gu** *University of Florida*
Many-body localization in random-anisotropy $S=1$ chain and possible realization in doped organo-metallic quantum magnets
- Frank Hagelberg** *East Tennessee State University*
Giant magnetoresistance in transition metal dichalcogenide monolayers
- Jun Jiang** *University of Florida*
Modeling and structure analysis of amorphous and doped Ta_2O_5 for low mechanical loss coatings
- Takashi Kawakami** *RIKEN Center for Computational Science*
Electronic structures of $CaMn_4O_5$ cluster in oxygen evolving complex of photosystem II. Theoretical calculations by LPNO-CC methods in the S_1 state of the Kok cycle
- Shuanglong Liu** *University of Florida*
Electric field effects on magnetism in CrI_3 bilayers
- Shubin Liu** *University of North Carolina*
Quantification and origin of cooperativity: Insights from density functional reactivity theory
- Svetlana Malinovskaya** *Stevens Institute of Technology*
Enhanced CARS for remote detection
- Alec Mishkin** *University of Florida*
Generating amorphous structures by combining reverse Monte Carlo and molecular dynamics and analyzing with graph theory algorithm
- Haechan Park** *University of Florida*
First principles study of magnetism in bilayer manganese phthalocyanine
- Luis Abel Puerta Silva** *Universidad de Carabobo*
Molecular descriptor to classify the different isomers of cocaine
- Kizashi Yamaguchi** *RIKEN Center for Computational Science*
Theoretical elucidation of the $Si(i=0-3)$ intermediates and transition state (S_4) in the Kok cycle for photosynthetic water oxidation; comparisons with the serial femtosecond crystallography (SFX)
- Maher Yazback** *University of Florida*
DFT study of the magnetic and structural properties of the DTN molecular crystal
- Zhuo Ye** *Iowa State University*
First-principles calculation of correlated electron materials based on Gutzwiller wave function beyond Gutzwiller approximation
- Jiexiang Yu** *University of Florida*
Magnetic interactions in covalently linked $[Mn_3]$ -dimer single-molecule magnets

PLENARY 5 - RELATIVISTIC QUANTUM MECHANICS
8:30AM-10:30AM

Chair: Mark Pederson

U.S. Department of Energy

Kenneth Ruud

University of Tromsø

All-electron fully relativistic Kohn–Sham theory for solids using Gaussian-type basis functions

Gustavo Aucar

Universidad Nacional del Nordeste

Relativistic quantum chemistry and polarization propagators theoretical grounds, some novel physical insights and recent applications

Kirk Peterson

Washington State University

Progress in correlation consistent basis sets for heavy elements – from transition metals to transactinides

PLENARY 6 - SEARCH FOR NOVEL MAGNETIC SYSTEMS
10:50AM-12:50PM

Chair: Hai-Ping Cheng

University of Florida

Kyungwha Park

Virginia Tech

Multireference ab initio studies of magnetic properties of TbPc₂-type single-molecule magnets

Grace Morgan

University College Dublin

Electronic and structural order parameters in Mn³⁺ metal-organics with S=1 to S=2 spin state switching

Jia Chen

University of Florida

Molecular model for Chevrel phase superconductivity

PLENARY 7 - BIG DATA AND MACHINE LEARNING
2:30PM-4:30PM

Chair: Jaochim Sauer

University of California, Irvine

Francesca Tavazza

National Institute of Standards and Technology

K-point integration: An example of how controlled approximations introduce uncertainty in DFT

Eric Isaacs

Northwestern University

Data-driven design of electronic band structure for materials

Adrian Roitberg

University of Florida

Neural networks learning quantum chemistry: The rise of the machines

≡ THURSDAY, FEBRUARY 21, 2019 ≡

PLENARY 8 - QUANTUM COMPUTING
4:45PM-6:45PM

Chair: Roland Lindh

Uppsala University

Sabre Kais

Purdue University

Quantum computing for complex chemical systems

James Freericks

Georgetown University

A primer on quantum computing for the condensed matter theorist

Jiri Pittner

Czech Academy of Sciences

Towards quantum chemistry on quantum computers

≡ FRIDAY, FEBRUARY 22, 2019 ≡

PLENARY 9 - THEORY AND METHODS FOR THERMOELECTRICS
8:30AM-10:30AM

Chair: Hendrik Monkhorst

University of Florida

George Nolas

University of South Florida

Thermoelectrics: A look back so we can move forward towards new materials developments

David Singh

University of Missouri

Contradictory transport requirements for high ZT and their resolution

Valdan Stevanovic

Colorado School of Mines

On a quest for novel thermoelectric materials: Theory and computation guided discovery and design

PLENARY 10 - THEORY AND METHODS FOR MAGNETISM
10:50AM-12:50PM

Chair: Xiaoguang Zhang

University of Florida

Qian Niu

University of Texas

Geometric effects on orbital magnetism

Guo-Ping Zhang

Indiana State University

Femtosecond laser-induced demagnetization: Femtomagnetism

Alex Zunger

University of Colorado Boulder

Description of paramagnetism, gap formation and atomic displacements in 3D oxide perovskites in polymorphous DFT

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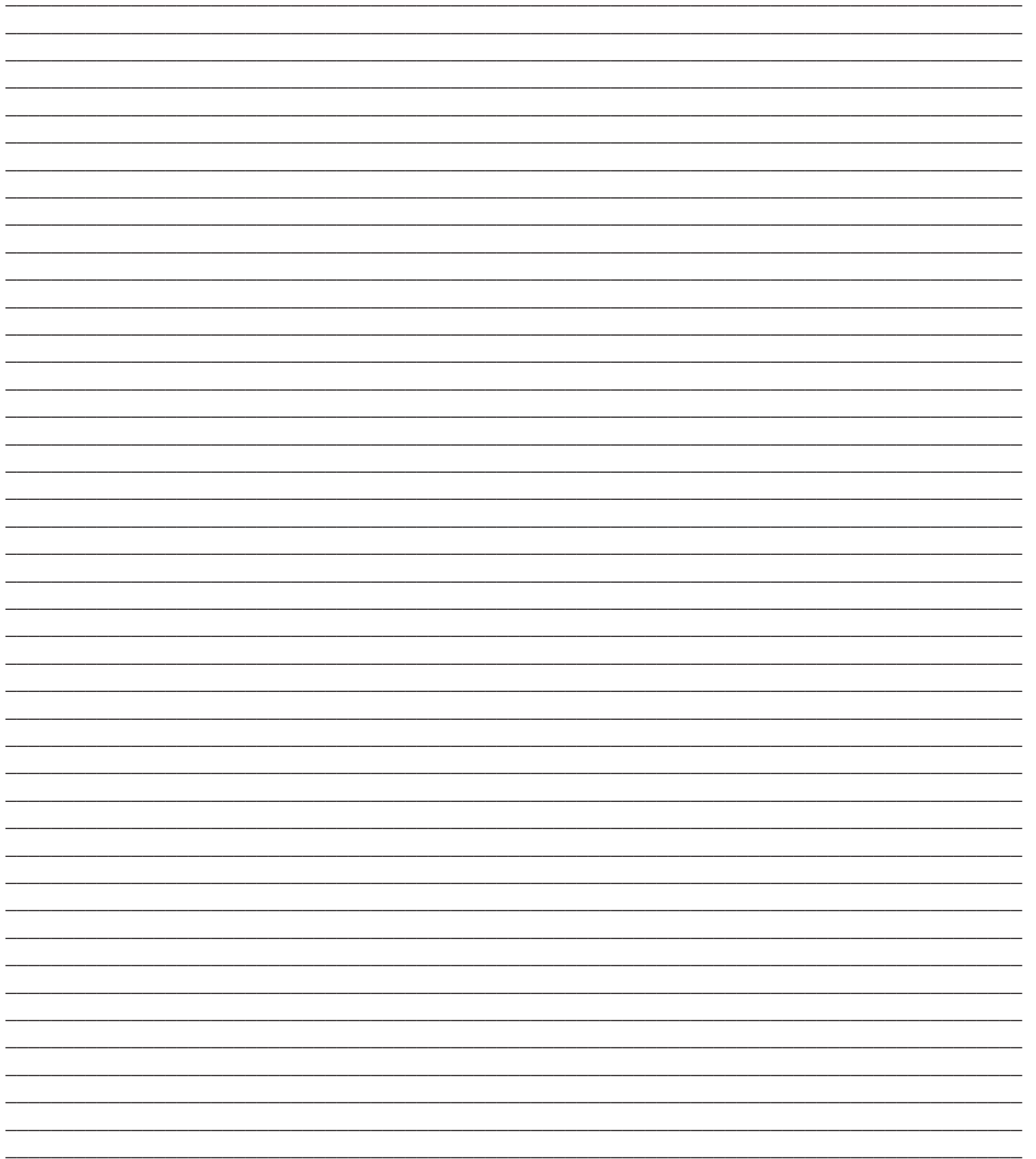
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