



ACS DIVISION OF PHYSICAL CHEMISTRY
255th NATIONAL MEETING
New Orleans, Louisiana
18-22 March 2018

THEME: *Nexus of Food, Energy, and Water*

CALL FOR PAPERS



The Division of Physical Chemistry has organized the following topical oral symposia, consisting of both invited and contributed papers, as well as a general poster session. **The abstract submission deadline is 16 October 2017.** For those interested in an oral presentation, please submit abstracts to the appropriate symposium. For each symposium, the organizers (listed below) will select some contributed papers for oral presentations; contributions not selected for oral presentations will be assigned to the poster session.

**QUANTUM CHEMICAL PROGRAM DEVELOPMENT IN A MODERN
COMPUTER AND PROGRAMMING ENVIRONMENT**

The focus of this symposium is on high performance computing, but more specifically on novel computer architectures and the exascale—as well as how chemists can (or cannot) make effective use of the new and anticipated advances. We will be soliciting contributions in the following topical areas: (a) towards exascale computing, (b) parallel environments, (c) new programming languages and domain specific languages and code generators, (d) new hardware solutions, and (e) software engineering practices.

Roland Lindh, *Uppsala University*, roland.lindh@kemi.uu.se

Anna Krylov, *University of Southern California*, krylov@usc.edu

Mark Gordon, *Iowa State University*, mark@si.msg.chem.iastate.edu

Theresa Windus, *Iowa State University*, twindus@iastate.edu

**CHIRALITY FROM MOLECULES TO MATERIALS: ADVANCES IN
EXPERIMENT AND THEORY**

Chirality always has played a fundamental role in chemistry, since most biologically relevant molecules are chiral and Nature has “selected” only one enantiomer to be part of living organisms. In recent years, interest in chiral compounds also has extended to inorganic systems, where chiral metal complexes and supramolecular frameworks are used to design and build complex materials having applications in electronics and sensing. Despite extensive efforts since the first studies of chirality early in the 19th century, many questions remain unanswered, such as what determines the chiroptical response of a compound (i.e., optical activity) and how can these properties be predicted from first principles. This symposium will bring together leading experimental and theoretical scientists engaged actively in the investigation of chiral systems from a variety of different viewpoints, including molecular synthesis and characterization taking place in diverse environments. The meeting will cover fundamental as well as applied aspects of research on chiral molecules and materials, thus providing a unique venue to discuss state-of-the-art developments in this multifaceted field.

Marco Caricato, *University of Kansas*, mcaricato@ku.edu

Patrick Vaccaro, *Yale University*, Patrick.vaccaro@yale.edu

COLD MOLECULES FOR CHEMISTRY

This symposium presents an overview of recently developed molecular cooling techniques and applications of the resulting cold molecular gases for chemistry. Cold molecular gases offer a range of exciting opportunities that are enabled by cooling the molecular motion and controlling the internal quantum degrees of freedom. Recent advances in cooling schemes overcome many complications due to the large number of internal modes, allowing high-efficiency production of cold molecules that opens the door to exploration of novel chemistry at ultra-low temperatures. Trapping of cold molecules also allows extended interaction times for collision and reaction studies. The near-zero kinetic energy of a cold molecular gas means that the macroscopic properties are dominated by the microscopic interactions between molecules. This will allow arrays of molecules to be assembled in a controllable and additive manner, to make “quantum lego” structures for performing controlled quantum simulation of quantum chemistry, materials, and dynamics. This symposium brings together quantum chemists and physicists to foster discussions on the new applications of cold molecules for chemistry.

Kang-Kuen Ni, *Harvard University*, ni@chemistry.harvard.edu

K. Birgitta Whaley, *University of California, Berkeley*, whaley@berkeley.edu

**ADVENTURES IN DENSITY FUNCTIONAL THEORY:
A SYMPOSIUM IN HONOR OF MEL LEVY AND JOHN PERDEW**

Over the past thirty years, density functional theory has emerged as the default method for quantum chemistry calculation, mainly because it often provides adequate accuracy at moderate computational cost and because it can be generally used as a black-box method, with little need to adjust parameters. However further progress beyond the commonly used approximations has been challenging. The proposed symposium is designed to provide a perspective on the current status of density functional theory (DFT), with emphasis on (1) understanding the fundamental nature of (and obstacles to) accurate density functional approximations and (2) the exposition of creative new approaches to DFT. We are particularly interested in contributions that address questions like the following: What are the main obstacles to developing more accurate and/or more robust density functional approximations? What new types of problems should we be considering? What new domains of application for DFT are emerging? What types of approaches are promising (or futile)?

Adventures in Density Functional Theory: Robert Ghormley Parr Memorial Symposium

Professor Parr guided the evolution of quantum chemistry from the primordial era to the present. His impact on science -- through his own scientific work, the work he shepherded through his group (much of which he refused to claim co-authorship), the many scientists he selflessly taught, mentored, and supported, and his own exemplary scientific life and temperament -- is immeasurable. This “symposium within a symposium” will feature frontier research developments in density functional theory.

Paul Ayers, *McMaster University*, ayers@mcmaster.ca

Weitao Yang, *Duke University*, weitao.yang@duke.edu

**QUANTUM CHEMISTRY, DYNAMICS AND REACTION MODELING
FOR MOLECULES AND MATERIALS IN ASTROPHYSICAL
ENVIRONMENTS**

Over 200 different molecules have been identified in various astrophysical environments. Chemical theorists contribute in many ways to the identification and understanding of this chemical complexity by supporting and sometimes guiding the efforts of experimentalists and observers. Using quantum chemistry, molecular dynamics, reaction rate theory, and sophisticated reaction network modeling programs, theorists (i) predict spectra of gas phase molecules and condensed phase model systems as well as dipole moments and other response properties, (ii) characterize reactions, and (iii) model the time-dependent composition and physical properties of solar and extrasolar atmospheres, interstellar clouds, and protoplanetary disks. Although the symposium focuses on theory, experimentalists and observers are invited to challenge the theorists to provide assistance in their work that would otherwise not be possible.

David Woon, *University of Illinois*, davidwoon@gmail.com

Herma Cuppen, *Radboud University*, h.cuppen@science.ru.nl

**UNDERSTANDING THE COMPLEXITY OF THE NANO/BIO
INTERFACE WITH EXPERIMENT AND COMPUTATION**

This symposium highlights recent advances in understanding the physical forces governing the behaviors and properties of nano-bio interfaces. Topics include quantitative analysis of biomolecular structure at interfaces and the resulting reactions, as well as methods development. In particular, non-equilibrium interactions are of interest, as well as complexity that spans multiple space and time scales. There will be a focus on new imaging and spectroscopic analytical insights, and both experimental and computational contributions are included within the scope of this symposium.

Franz Geiger, *Northwestern University*, f-geiger@northwestern.edu

Christy Landes, *Rice University*, cflandes@rice.edu

PHYSICAL CHEMISTRY OF IONIC LIQUIDS

From applications in energy sciences to advanced materials and technologies, ionic liquids continue to attract intense interest due to their unusual and advantageous properties. Over the last decade, physical chemistry has played a dominant role in explaining how ionic liquids work and how they can be employed in critical applications. This symposium will present the most recent experimental and computational viewpoints on ionic liquids' intrinsic dynamics, nano- and meso-structures, interfacial phenomena, solvation, physical properties, and nanoscience, as well as their uses in electrochemistry, catalysis, separations, biomass utilization, energy, and other applications. Co-sponsored by the Division of Colloid and Surface Chemistry.

Edward W. Castner, Jr., *Rutgers University*, ecastner@chem.rutgers.edu

Edward J. Maginn, *University of Notre Dame*, ed@nd.edu

Claudio J. Margulis, *University of Iowa*, claudio-margulis@uiowa.edu

Scott K. Shaw, *University of Iowa*, scott-k-shaw@uiowa.edu

James F. Wishart, *Brookhaven National Laboratory*, wishart@bnl.gov

ENERGY AND CHARGE TRANSFER AT NANOSCALE INTERFACES

Understanding the fundamental factors that guide energy and charge transfer at nanoscale interfaces is crucial to the optimization of next generation energy devices, catalysts, and sensors. To this aim, developing new experimental and theoretical techniques that break the boundaries with which we temporally and spatially resolve dynamics at nanoscale interfaces can reveal new insights into how to structurally design junctions that efficiently control the flow of energy and charge. Although ultrafast spectroscopy can now routinely view processes occurring on femtosecond timescales and super-resolution microscopy can reveal objects smaller than the diffraction limit of light, only recently have experimentalists started to explore techniques that simultaneously couple high time and spatial resolution. This symposium will bring together spectroscopists, microscopists, theorists, and other researchers working on problems wherein interfacial charge and energy transfer is critical. By gathering researchers that employ a wide range of technologies and approaches to study nanoscale interfaces, we hope to foster collaborative efforts that can speed the development of new time-resolved microscopies and theoretical approaches that can reveal electronic dynamics at these crucial junctions.

Libai Huang, *Purdue University*, libai-huang@purdue.edu

Sean T. Roberts, *University of Texas at Austin*, roberts@cm.utexas.edu

Katherine A. Willets, *Temple University*, kwillets@temple.edu

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the general poster session to be held on Wednesday evening, 21 March 2018. See announcement below for information about the Physical Chemistry Student Poster Awards.

Michael A. Duncan, *University of Georgia*, maduncan@uga.edu

On-Line Abstract Submission Deadline: 16 October 2017
<http://abstracts.acs.org>

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

Six awards with monetary prizes will be awarded for posters presented by students during the Physical Chemistry Poster Session on Wednesday evening, March 21. To be eligible for the awards, the **presenting author** must be a graduate or undergraduate student at the time of the poster presentation and must be present during judging.

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