ACS DIVISION OF PHYSICAL CHEMISTRY

FALL 2023 NATIONAL MEETING

THEME: Harnessing the Power of Data

13-17 August 2023 ◆ San Francisco, California

CALL FOR PAPERS

The Division of Physical Chemistry (PHYS) is hosting the following ten oral symposia, consisting of both invited and contributed papers, as well as a general poster session. **Abstract submission will open on January 9 and remains open until April 4**. For those interested in an oral presentation, please submit abstracts to the appropriate symposium via ACS-MAPS. 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.

Chemical Bonding Theory – Perspectives from Valence Bond (VB) Related Theories

Most fundamental concepts in chemistry originate from the early qualitative valence bond (VB) theory, including bond pairs, lone pairs, hybrid orbitals, and resonance. However, the computational complexity involving the non-orthogonality of the orbitals in VB theory hindered its further development and over the years MO theory (including DFT) has become synonymous with computational chemistry. During the past two to three decades, there has been a remarkable renaissance in modern ab initio VB or similar methods along with critical computer software developments and distributions. The broad applications of these VB methodologies have generated novel insights into the nature of chemical bonding and reaction mechanisms and enriched our understanding of chemistry. Thus, VB methods complement the popular MO/DFT methods in a multitude of ways. Considering the recent remarkable advances in VB theory and its applications, we have organized a symposium that will highlight the work of the major players in the VB field, as well as leading experts in electronic structure and chemical bonding theories, who will showcase their research findings, create consensus from different perspectives, and, finally, draw advancements in VB theories to the attention of the whole chemistry community. The organizers welcome other submissions that contribute to these themes.

Thom H. Dunning, University of Washington, *thdjr@uw.edu*
John M. Galbraith, Marist College, *John.Galbraith@marist.edu*
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Marine Aerosols in the Atmosphere and Their Impacts

Sea spray aerosol particles (SSA), formed through wave breaking at the ocean surface, contribute to natural aerosol particle concentrations in remote regions of Earth's atmosphere and alter the direct and indirect effects of aerosol particles on Earth's radiation budget. The proposed symposium will focus on how physical chemistry plays a key role in understanding these global impacts. The symposium will be co-organized by researchers and leaders within the National Science Foundation (NSF) Center for Aerosol Impacts on Chemistry of the Environment. As one of the NSF Centers for Chemical Innovation (CCI), CAICE tackles the grand challenge of elucidating how the chemical complexity of atmospheric aerosol particles impacts our atmosphere and climate. SSA has tremendous chemical variability depending on ocean chemistry, biology, and physical factors such as waves and wind. CAICE has established a unique ocean-atmosphere interaction facility that replicates natural sea spray aerosol in a controlled setting, allowing for detailed fundamental physical chemistry studies of aerosol reactions in both complex "top-down" and building the complexity "bottom-up" approaches. A hallmark of this research has been the tight coupling of theory and experiment. Outreach and educational activities have also played a key role in getting K-12 students and the public excited about environmental and physical chemistry. This symposium celebrates the exciting and fruitful 13 years as this chapter of the NSF CCI comes to a close.

Tim Bertram, University of Wisconsin-Madison, *tbertram@chem.wisc.edu*
Vicki Grassian, University of California, San Diego, *vhgrassian@ucsd.edu*
Christopher Lee, University of California, San Diego, *leechris@ucsd.edu*
Kimberly A. Prather, University of California, San Diego, *kprather@ucsd.edu*

Chemistry and Properties of Two-Dimensional Materials

Two-dimensional (2D) materials have spawned a new frontier in chemistry and materials research. While graphene was the primary focus of study in the early days of 2D materials research, today many new classes of 2D materials have captivated the interest of physicists, chemists, engineers, and materials scientists. In order to provide a comprehensive and critical perspective on the status of 2D materials, this symposium aims to (i) highlight emerging research, (ii) cultivate a diverse community of scholars, and (iii) provide a roadmap for future research opportunities. Talks in this symposium cover elemental 2D materials beyond graphene (e.g., phosphorene, borophene, silicene), compound 2D materials (e.g., transition metal chalcogenides), layered metal oxides and halides, organic-inorganic metal halide layered perovskites, 2D molecular frameworks, and their heterostructures, including moire superlattices. The symposium welcomes submissions that focus on the synthesis, fundamental properties, device physics studies, and applications of these materials, for example in quantum information, sensing, optics, and energy conversion. Contributions focused on development of methods for controlled growth of 2D materials and on advanced spectroscopy and microscopy techniques are of particular interest. Bringing together researchers with complementary expertise in advanced spectroscopy, microscopy, synthesis, device fabrication, and application of 2D materials promises to open new frontiers for 2D materials in the world of chemistry.

Sarah B. King, University of Chicago, *sbking@uchicago.edu*
Thomas Kempa, John Hopkins University, *tkempa@jhu.edu*
Archana Raja, Lawrence Berkeley National Laboratory, *araja@lbl.gov*

Optical Spectroscopy and Microscopy Across Biological Scales

Optical spectroscopy and microscopy have allowed investigations of the complex biological structures and dynamics across different scales with unprecedented precision in space, time, and function. This symposium will bring together experimentalists and theorists with various spectroscopic and microscopic specialties ranging from nonlinear spectroscopy to single-molecule spectroscopy; from fluorescence imaging to Raman/IR or other label-free modalities; from fundamental biophysics on protein dynamics to investigations on the live cell, neuron and animal levels; and across different career stages to discuss the recent technical and application advances and brainstorm key issues and questions.

Gabriela Schlau-Cohen, Massachusetts Institute of Technology, *gssc@mit.edu*
Lu Wei, California Institute of Technology, *lwei@caltech.edu*

Quantum Computing for Tackling Challenges in Quantum Chemistry

Quantum computing is a fundamentally new paradigm for computation and information processing made possible by harnessing physical phenomena unique to quantum mechanics. Chemistry is one of the most promising applications of quantum computing. While the current noisy near-term quantum computing systems fall short of the requirements for fault-tolerant systems, they provide unique opportunities for novel quantum applications in chemistry. This symposium will bring together a diverse community of scientists from industry, academia, and government to identify challenges in chemistry simulations with classical computers and share the newest developments and solutions brought by quantum computers.

Bert de Jong, Lawrence Berkeley National Laboratory, *wadejong@lbl.gov*
Rosa Di Felice, University of Southern California, *difelice@usc.edu*
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James D. Whitfield, Dartmouth University, *james.d.whitfield@dartmouth.edu*

Data-Driven Design of Energy Materials

The past years have been marked by fast-paced advances in the data-driven and Machine Learning (ML)-aided design and characterization of energy materials. Equally remarkable is the broad range of theoretical methods, physical systems, and applications that ML-aided research has enabled to explore. Recent advances in the field include the design of high-performance materials for energy storage, the modeling of catalysts for renewable energy, combinatorial approaches for ceramic fuel cells, combined quantum mechanical-ML approaches for electrochemical systems, and the design of novel nanoporous materials for hydrogen capture, among others. This symposium will bring together chemists, physicists, and engineers from these different areas, with complementary computational and experimental expertise, to share the cutting-edge advances in the design of energy materials enabled by ML in their respective fields. We anticipate that the symposium will enable participants to explore how recent methodological developments can be transferred from one area to another, and, in turn, accelerate discovery and address outstanding challenges in energy materials research.

Jerome Delhommelle, University of Massachusetts, Lowell, *Jerome_Delhommelle@uml.edu*
Mingda Li, Massachusetts Institute of Technology, *mingda@mit.edu*
Fang Liu, Emory University, *fang.liu@emory.edu*

The Astrochemistry Subdivision: A Decade of Progress and Prospects for the Next Decade

The Astrochemistry Subdivision convened its first symposium 10 years ago during the Fall 2013 national meeting. It has been a decade of immense progress for the field of astrochemistry, and many members of the Subdivision have made seminal contributions to the field. The astronomical detection of new molecules has exploded in recent years with the Atacama Large Millimeter Array (ALMA) and large single-dish observatories (e.g., GBT, IRAM 30m) leading the way. 2021 alone saw announcements for the detection of over 30 new molecules, far more than the annual averages from the previous years. The James Webb Space Telescope has already sent back stunning imagery of the cosmos. All observations are founded upon critical experimental and theoretical chemistry contributions, which provide a steady stream of data and predictions. Observation, experiment, and theory all complement each other enormously. As a symposium that looks both back over the accomplishments of the last decade and forward toward the prospects of the next decade, we will encourage our speakers to share their dreams and ambitions for what might be learned in the years to come.

Olivia H. Wilkins, NASA, *olivia.h.wilkins@nasa.gov*
David W. Woon, University of Illinois Urbana-Champaign, *davidewoon@gmail.com*

Intersections of Climate, Urban Living, and Chemistry

The Earth is warming. Patterns of rainfall are changing. Urban life is becoming increasingly electrified. As a result of these three intersecting trends there are profound changes occurring in the atmospheric composition of cities. For example, emissions from restaurants, household cleaning solvents, and urban trees are overtaking emissions from vehicles as one of the dominant factors contributing to poor air quality. Many of these emissions are strongly temperature dependent, making air quality especially poor on the hottest days. In addition, as emissions decrease, disparities in exposure to poor air quality that reflect land use policy are becoming more evident. In this symposium, we invite contributions that address this changing landscape, including laboratory and field based observational studies, evaluation of mechanisms and assessment and prediction with numerical models.

Steven S. Brown, National Oceanic and Atmospheric Administration, *steven.s.brown@noaa.gov*
Ron C. Cohen, University of California, Berkeley, *rccohen@berkeley.edu*

NMR and MRI for Materials Characterization

Nuclear magnetic resonance spectroscopy and imaging are important techniques for understanding structures, dynamics, and spatial distributions of atoms and molecules within functional materials. The insights gained from these techniques have led to immense improvement of functional properties and guided materials discovery and design. This symposium will highlight recent developments in NMR and MRI and their applications in advanced materials characterizations, with a focus on five key topical areas: (1) New Methods and Hyperpolarization; (2) NMR and MRI of Energy Materials; (3) Polymers and Soft Matter; (4) Nanomaterials and Semiconductors, and Quantum Materials; and (5) Porous Materials and Catalysts.

Leah B. Casabianca, Clemson University, *lcasabi@clemson.edu*
Yan-Yan Hu, Florida State University, *yhu@fsu.edu*
Louis A. Madsen, Virginia Tech, *lmadsen@vt.edu*
Aaron J. Rossini, Iowa State University, *arossini@iastate.edu*
Kay Saalwächter, Martin Luther University Halle-Wittenberg, *kay.saalwaechter@physik.uni-halle.de*

Symposium in Honor of Marsha I. Lester

Marsha I. Lester, the Christopher H. Browne Distinguished Professor in the Department of Chemistry at the University of Pennsylvania, has long been a leading figure in experimental chemical physics. She has developed innovative methods for generating and characterizing a variety of open-shell complexes and reactive intermediates, enabling her to map out previously uncharted regions of chemical reaction space. In honor of Marsha Lester's work, this symposium will bring together experimental and theoretical colleagues at the forefront of a wide-spanning scope of topics within gas phase chemical dynamics.

Nathanael M. Kidwell, College of William and Mary, *nmkidwell@wm.edu*
Stephen J. Klippenstein, Argonne National Laboratory, *sjk@anl.gov*
Julia Lehman, University of Birmingham, *j.lehman@bham.ac.uk*
Anne B. McCoy, University of Washington, *abmccoy@uw.edu*

YOUNG INVESTIGATOR RESEARCH AWARDS

Our PHYS Division Young Investigator Research Award talks will be presented during the relevant PHYS technical symposia. See http://phys-acs.org/young-investigator-award-phys/ for application information.

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session. Multiple awards will be given for exemplary work. 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.

On-Line Abstract Submission Deadline: 4 April 2023
http://abstracts.acs.org

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