ACS DIVISION OF PHYSICAL CHEMISTRY
257TH NATIONAL ACS MEETING
Orlando, Florida March 31 to April 4, 2019

Meeting Theme: "Chemistry for New Frontiers"

CALL FOR PAPERS

The Division of Physical Chemistry has organized the following topical oral symposia, consisting of both invited and contributed papers.
The abstract submission window opens 20 August and closes on 29 October 2018. 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.

ADVANCES IN DATA COLLECTION AND ANALYSIS OF BIOMOLECULAR STRUCTURES

This symposium will highlight recent advances in a broad range of experimental techniques and computational modeling, foster cross-disciplinary discussions, and drive forward the active development on an emerging field of integrative, multi-technique structural biology and biophysics. Particular focus will be placed on the latest development in (a) experimental data acquisition (e.g., FRET, NMR, SAXS, EM, protein footprinting, H/D exchange, cross-linking), and (b) computational modeling that enables the combination of multiple sources of experimental structural data. Both development and application of such multi-technique modeling toward challenging topics such as protein-protein interaction, macromolecular assembly, and protein disorder, are particularly encouraged. By emphasizing the synergy between computation and experiment, this symposium will promote collaborative dialogues for both methodological development and broader dissemination for years to come.
Sichun Yang, *Case Western University*, sxy227@case.edu
Steffen Lindert, *The Ohio State University*, lindert.1@osu.edu

EMERGING FRONTIERS IN FLUORESCENCE MICROSCOPY: FROM SINGLE MOLECULES TO SUPER RESOLUTION

Single-molecule imaging and super-resolution microscopy have transformed our ability to interrogate the dynamics and nanoscale organization of complex biological and materials systems. These innovations have been fueled by a range of technical advances in optical engineering, fluorescent probes, image processing algorithms, device fabrication, and sample processing techniques. This symposium will focus broadly on topics in single-molecule imaging and super-resolution microscopy, including recent technical breakthroughs and scientific applications in biochemistry, biophysics, molecular biology, cell biology, catalysis, and materials science.
Tae-Hee Lee, *Pennsylvania State University,* txl18@psu.edu
Joshua C. Vaughan, *University of Washington,* jcv2@uw.edu

PRODUCING EQUILIBRIUM AMORPHOUS PACKINGS

Producing equilibrium amorphous packings at low temperatures requires thousands of years of aging of a liquid-quenched glass, as rapidly increasing barriers to relaxation arise when the temperature of a super-cooled liquid is decreased well below its melting point. Recent advances in experiments and computer modeling have enabled new methods to overcome these barriers and produce equilibrated low-energy packings in reasonable timescales. For example, stable molecular, atomic, and colloidal glasses have been made by exploiting the unusual surface mobility of glasses in vapor-deposition experiments; simulations have used changes to the dynamical rules (as in swap Monte Carlo algorithms) to equilibrate bulk liquids at temperatures previously thought to be completely inaccessible to numerical studies. The ability to produce these low-energy states provides an opportunity to produce materials with interesting mechanical, optical, and electronic properties, and also enable direct comparisons with predictions of different theoretical models of glassy states. This session aims to highlight recent experimental and theoretical advances in producing stable amorphous packings and discuss their unique material properties.
Zahra Fakhraai, *University of Pennsylvania*, fakhraai@sas.upenn.edu
Daniel Sussman, *Syracuse University*, dmsussma@syr.edu

QUANTUM EMBEDDING ELECTRONIC STRUCTURE METHODS

Embedding is a trending topic in quantum chemistry and related disciplines. In an effort to achieve ab-initio approaches to multi-scale modeling, research groups in chemistry and physics are developing a rich family of electronic structure methods having as ultimate goals the description of strongly-correlated electronic systems, realistically-sized systems and generally the expansion of the applicability of currently available ab-initio electronic structure methods. The symposium will span a closely linked yet wide array of topics: from density embedding and wavefunction-in-DFT embedding to density matrix and Green function embedding, including dynamical mean-field theory in DFT (DMFT in DFT). The symposium will highlight contributed and invited talks by theoretical chemists, physicists, and engineers whose work focuses on the theoretical foundations of embedding methods as well as their implementations in fast computer codes that exploit modern computational architectures and afford broad applicability.
Michele Pavanello, *Rutgers University*, m.pavanello@rutgers.edu
Adam Wasserman, *Purdue University*, awasser@purdue.edu

FRONTIERS IN VIBRATIONAL SPECTROSCOPY: EXPERIMENTS AND THEORY

This symposium will highlight the chemical insights obtained from vibrational spectroscopy. Emphasis will be placed on new experimental and theoretical/computational approaches that genuinely explore new frontiers in this relatively established discipline. Topics of interest include tracking chemical reactions via ultrafast vibrational spectroscopy, determining the structure(s) of molecules and clusters using highly resolved vibrational spectroscopy, probing the dynamics of coupled electronic and nuclear motions, extracting thermodynamic information from vibrational spectra, characterizing low-frequency and large-amplitude motions, and developing or applying new theoretical approaches for predicting and analyzing vibrational spectra. The slate of speakers will generate lively discussions at the interface of experiment and theory, with the intent of clarifying—and possibly defining—new future directions in vibrational spectroscopy.
Etienne Garand, *University of Wisconsin*, egarand@wisc.edu
Ryan P. Steele, *University of Utah*, ryan.steele@utah.edu

MATERIALS AND TECHNIQUES TO ADVANCE REDOX FLOW BATTERIES

Inexpensive electrical energy storage is critical for successful transformation of the electric grid. The redox flow battery is a promising grid storage technology with an architecture that enables decoupling of power and energy, extended lifetimes, and simplified manufacturing. While some large-scale installations of flow batteries are in operation, the costs of commercial systems are too high to allow for universal adoption. This symposium will offer a broad view of recent development of electrode materials and electrolyte components for redox flow batteries. Topics of interest include, but are not limited to, advances in organic or metal coordination complexes, electrolyte formulations, electrode engineering, separator and membrane design, flow cell analysis as well as development in electrochemical diagnostic techniques. Beyond learning of recent trends in the field, the 8-session symposium aims to begin building consensus around best practices in materials screening and cell design and cycling.
Susan Odom, *University of Kentucky*, susan.odom@uky.edu
Fikile Brushett, *Massachusetts of Technology*, brushett@mit.edu

SUSTAINABLE SOFTWARE FOR COMPUTATIONAL MOLECULAR SCIENCE

The field of computational molecular sciences (CMS) broadly encompasses quantum chemistry, materials science, and biomolecular simulation. Modern molecular dynamics and quantum chemical models have achieved such a level of robustness and accuracy that they are often considered "computational experiments," with direct impact on applications such as the design of more efficient combustion systems, development of new chiral drugs, and many others. These scientific breakthroughs have been made possible by the evolution of hundreds of community codes, some with lifetimes reaching back to the earliest days of computing. Recently, a "software revolution" has begun to grow as more and more molecular scientists adopt the tools, methods, and even philosophy of modern software engineering. This symposium will highlight recent advances in software for CMS, and will include topics such as reaching advanced hardware, reproducibility, software tools for machine learning, and best practices in software development.
Jessica Nash, *Molecular Sciences Software Institute (VT)*, janash@vt.edu
Eliseo Marin-Rimoldi, *Molecular Sciences Software Institute (VT)*, meliseo@vt.edu
Daniel G. Smith, *Molecular Sciences Software Institute (VT)*, dgasmith@vt.edu
Daniel Crawford, *Virginia Tech and the Molecular Sciences Software Institute*, crawdad@vt.edu

MODELING DYNAMICS IN DENSE MANIFOLDS OF ELECTRONIC STATES

Practical theoretical protocols for modeling nonadiabatic dynamics on the lowest few electronic states of molecules and materials are now widely used and have yielded many important insights into a range of chemical phenomena. Modeling nonadiabatic dynamics in systems that explore dense manifolds of electronic states, however, remains an open challenge in theoretical chemistry. The development of robust methods for modeling dynamics in dense manifolds of electronic states would expand the capability of theory in a wide range of fields, for example atmospheric chemistry, astrochemistry, molecules in strong laser fields, radiation damage, and optoelectronic and plasmonic materials. Theorists in these disparate application domains face similar theoretical challenges. Our symposium brings together chemists and physicists from these different application areas to examine the most fruitful developments in the modeling of electronic and nonadiabatic dynamics in dense manifolds of electronic states, to explore how developments in one area of chemistry can be leveraged in others, and to discuss recent progress towards answering pressing chemical questions in the above areas.
Benjamin G. Levine, *Michigan State University*, levine@chemistry.msu.edu
Petr Slavíček, *University of Chemistry and Technology, Prague***,** Czech Republic, petr.slavicek@vscht.cz

STRUCTURE AND DYNAMICS OF ELECTROLYTES: FROM THE BULK TO INTERFACES

The theme of this symposium is the characterization of the structure and dynamics, from the molecular to the mesoscale, in aqueous and non-aqueous electrolytes for energy storage. A substantial emphasis has been given to the development of new electrode materials, while design principles for liquid or gel electrolytes remain elusive. Soft matter, such as battery electrolytes, have short range order coupled to long range disorder. The transition in behavior as a function of length scale renders predictions and characterization challenging both in the bulk electrolyte and at crucial interfaces. The synergy between experiment and theory can bridge this knowledge gap. Moreover new approaches, both experimental and computational, linking temporal and spatial scales are essential. The proposed symposium will bring together experimentalists and theorists working with state-of-the-art methodologies to address the challenges of elucidating inherently multiscale processes. This symposium will be an excellent forum for engendering new collaborations along with the transfer of knowledge between experts working on different aspects of this broad area.
Ryan Jorn, *Villanova University*, ryan.jorn@villanova.edu
Revati Kumar, *Louisiana State University*, revatik@lsu.edu
Daniel Kuroda, *Louisiana State University*, dkuroda@lsu.edu

NEW FRONTIERS IN THE CONFLUENCE OF EXPERIMENTAL THERMODYNAMICS, STRUCTURAL INVESTIGATIONS AND THEORY/COMPUTATION

This symposium is organized by the Thermodynamics Consortium (https://www.thermocon.org) to bring together experimental materials scientists, chemists, geologists, computational, and structural scientists. Thermocon's goal is to provide an enhanced understanding of the fundamental thermodynamics of complex materials as well as how to apply this understanding to a rich variety of scientific and technological problems. It has already attracted a large and diverse scientific community (almost 300 international members) who are working together to change the way the academia, national labs, and industry interact. Thermodynamics forms the fundamental underpinning of reactivity, transformation, and stability. The needs of materials science, chemistry, earth and planetary science, and environmental science are both overlapping and complementary. The rapid developments in industry have resulted in an increasing need for improved and new materials, and better ways to study their properties. Thermocon welcomes both members and non-members to participate in the symposium to exchange ideas, start new collaborations, and ultimately bring the different fields closer together.
Kristina Lilova, *University of California, Davis*, kililova@ucdavis.edu
Nancy Birkner, *Duke University*, nancy.burkner@duke.edu
Di Wu, *Duke University*, d.wu@wsu.edu

PHYS WORKSHOP FOR UNDERGRADUATE CHEM MAJORS

The Workshop for Undergraduate Chemistry Majors is targeted for accomplished and research-active sophomore or junior chemistry majors who have enrolled in at least one semester of undergraduate physical chemistry. Up to 25 outstanding undergraduate chemistry students will be selected for a series of focused talks and social events during the Orlando ACS meeting. In addition, they will be expected to present posters on their research as part of the main PHYS poster session. More information and application materials can be found at http://phys-acs.org/ugrad_workshop/2019.html. The application deadline is October 15th.
Casey Londergan, *Haverford College*, ug-phys@haverford.edu

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday (3 April), from 6:00 to 8:00 PM. Up to six awards with monetary prizes 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: 29 October 2018 **http://abstracts.acs.org**

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