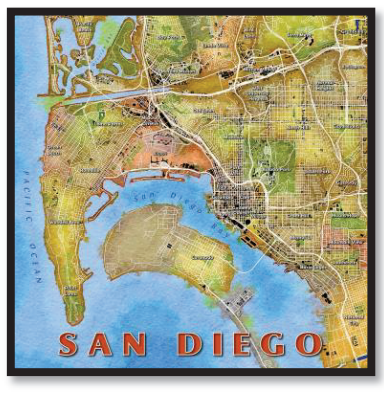
ACS DIVISION OF PHYSICAL CHEMISTRY
251st NATIONAL MEETING
THEME: Computers in Chemistry
13-17 March 2016 ◆ San Diego, California



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 topical and general poster sessions. Abstracts can be submitted online beginning August 15. **The abstract deadline is 12 October 2015**. 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.

Metastable Electronic States: Recent Advances In Theory and Experiment

Metastable electronic states play a key role in a wide range of processes including dissociative attachment, vibrational and electronic excitation of molecules, X-ray absorption, Coulomb decay, and photoinduced electron transfer, all of which present unique challenges for both experiment and theory. Although significant advances in theoretical and experimental characterization of metastable states have been made in recent years, major challenges still remain. This symposium will bring together theorists and experimentalists working on metastable states. Particular emphasis will be placed on the challenges of elucidating the dynamics and decay channels of metastable states of molecular systems.

Ksenia Bravaya, *Boston University, bravaya@bu.edu*
Kenneth D. Jordan, *University of Pittsburgh, jordan@pitt.edu*

Computer Simulations of Thermodynamics and Long-Time Kinetics of Molecular Events

The calculation of free energy landscapes and dynamical behavior are central to understanding biological behavior of macromolecular systems. Examples include protein folding, ligand binding, and the functioning of molecular machines. The well-known challenges inherent in long-time scale biomolecular calculations are spurring both hardware and algorithmic developments. The symposium will showcase recent advances in calculating free energy landscapes, pathways (mechanisms) and rates for the highly complex molecular processes underlying cell behavior. Method and algorithmic developments include transition path sampling, Markov state models, milestoning, transition path theory, weighted ensemble simulation, as well as adaptive and restraint-based free energy methods. Hardware advances include the development of special purpose machines, the exploitation of GPUs, and the utilization of massively parallel systems for molecular dynamics simulations.

Ron Elber, *University of Texas, ron@ices.utexas.edu*
Daniel M. Zuckerman, *University of Pittsburgh, ddmmzz@pitt.edu*
Ronald M. Levy, *Temple University, ronlevy@temple.edu*
Chung Wong, *University of Missouri-St. Louis, wongch@umsl.edu*

Supramolecular Aggregates: Fundamentals and Applications of Soft Self-assembled Materials

Supramolecular science is one of the most dynamic and interdisciplinary research areas, with potential for broad applications in a wide range of fields. This symposium offers a comprehensive view of recent research in the highly diverse field of self-assembled soft material systems. The aim of this symposium will be to link fundamental structural properties with physicochemical properties of supramolecular structures and to leverage fundamental knowledge for use in novel applications, which include the prediction and chemical design of self-assembling matter. This symposium will feature talks by cutting-edge scientists who will discuss their findings across length scales from atomic/molecular, to nano, micro, and macroscopic scales. Both experimental and theoretical topics will be covered.

Dorthe M. Eisele, *The City College of New York, eisele@ccny.cuny.edu*
Adam P. Willard, *Massachusetts Institute of Technology*, *awillard@mit.edu*

Decoding the Spectroscopic Signatures of Large Amplitude Motions: Challenges and Opportunities for Theory and Experiment

The symposium will highlight recent advances in experimental methods that provide increasingly clear spectroscopic observables for systems undergoing large amplitude motions, either due to zero-point motion in floppy modes or excitation to well-defined internal energy (or more recently, temperature). The patterns observed are usually not in line with readily available harmonic expectations. Therefore, advanced theoretical methods that accurately treat vibrational mode couplings and anharmonicities are essential in order to achieve quantitative understanding of the intricate dynamics and the interaction potentials that are encoded in the spectra. This symposium is largely concerned with vibrational spectroscopy of relatively small systems, floppy polyatomic molecules, weakly bound molecular clusters, and small molecules in nanoconfinement, that nonetheless exhibit sufficient complexity to express key paradigms that can also be accurately addressed with high-level theoretical methods. .

Mark A. Johnson, *Yale University*, *mark.johnson@yale.edu*
Zlatko Bačić, *New York University*, *zlatko.bacic@nyu.edu*

Electrochemistry at Solid/liquid Interfaces

Electrochemical interfaces are ubiquitous in nature and are present in a variety of technologies ranging from energy generation and storage to corrosion. Development of devices such as batteries, double layer capacitors, and fuel cells critically depends on understanding interfacial electrochemical phenomena and ability to tailor materials response, reactions and compatibility. Understanding of electrochemical interfaces and interfacial processes is challenging experimentally and computationally due to its complex and interdisciplinary nature. Computationally, it requires adequate representation of solid, liquid, and sometimes a glassy interfacial layer, which often exhibit disparate relaxation time scales and length scales (e.g., electronic, ionic, or more coarse grained descriptions). Experimentally, it requires in-situ techniques to probe the evolution of chemistry, structure, and properties at such a small length scale. This symposium will provide a discussion platform for modeling scientists and experimentalists to exchange ideas on development of novel methodologies and application of the existing methods to understanding structural properties, electrochemical reactions, transport processes under applied electric field at interfaces, as well as how these processes are coupled together.

Oleg Borodin, *Army Research Laboratory, oleg.a.borodin.civ@mail.mil*
Yue Qi, *Michigan State University*, *yueqi@egr.msu.edu*

Frontiers in Solar Light Harvesting Processes

The need for an affordable, clean, and abundant source of energy has generated vast amount of research in a variety of organic, inorganic and hybrid organic-inorganic nanostructured materials able to convert the solar energy into electricity or to store it chemically: conjugated polymers, quantum dots, semiconducting carbon nanotubes, transition metal complexes, hybrid perovskites and conventional semiconductors, to name a few. This symposium will address fundamental physical phenomena relevant to our understanding of advanced photo-electro-chemical energy conversion and storage in a broad variety of materials by bringing together experimentalists and theorists from different subfields.

Sergei Tretiak, *Los Alamos National Labs, serg@lanl.gov*
Todd D. Krauss, *University of Rochester, krauss@chem.rochester.edu*
Oleg V. Prezhdo, *University of Southern California, prezhdo@usc.edu*
Aditya Mohite, *Los Alamos National Labs, amohite@lanl.gov*

Physical Chemistry of Complex Environmental Interfaces

This symposium will provide a forum to explore the formation, composition, and reactions of aerosol particles (including aqueous droplets and ice) and their effect on atmospheric chemistry and climate. The meeting is motivated by the increasing realization that the surfaces of particles play a significant role in altering our climate, and only through a combination of theoretical, laboratory, and field studies can the impacts of aerosols on climate and the environment be understood and predicted. Presentations will focus on the key role that physical chemists can play in advancing our understanding of the chemical composition, morphology, and surface structure of atmospheric aerosol interfaces in their native state, how these particles form and grow, and how they control interfacial and multiphase reactions that influence local air pollution and global climate. As part of this symposium, we plan to hold an evening tour of a large-scale atmosphere-wave facility at the Scripps Institution of Oceanography for generating and investigating realistic, nascent sea spray aerosol.

Vicki Grassian, *University of Iowa, vicki-grassian@uiowa.edu*
Gilbert Nathanson, *University of Wisconsin, gmnathan@wisc.edu*

Structure And Dynamics in Enzymatic Catalysis Across Multiple Timescales: Experiment and Theory

"How enzymes work" is the topic of this cross-disciplinary symposium. It will explore where we've been, where we are, and where we need to go in our quest to fully understand the physical principles underlying enzymatic catalysis. The symposium will bring together experimental and theoretical investigators from a broad range of backgrounds who study enzyme dynamics across many time and length scales, from electronic and vibrational motions accessible by ultrafast spectroscopy to the slow conformational and structural changes relevant to active-site chemistry studied by high-resolution techniques. The symposium intends to highlight both cutting-edge experimental and theoretical work that aims at understanding the fundamentals of enzymatic processes.

Stefan Stoll, *University of Washington, stst@uw.edu*
Hannah S. Shafaat, *The Ohio State University, shafaat.1@osu.edu*

Physical Principles in Functional Nanoscience: A Symposium in Honor of Mostafa A. El-Sayed

This symposium will highlight cutting-edge advances in the understanding of the physical and chemical properties of noble metal and semiconductor nanostructures, the assembly of these nanostructures into functional materials, and the applications of these nanostructured materials in biomedicine, catalysis, photochemistry, and optoelectronics, areas that Prof. El-Sayed helped to shape. Focus will be on discussion of underlying physical principles that guide understanding and function.

Prashant K. Jain, *University of Illinois, Urbana-Champaign, jain@illinois.edu*
Christy Landes, *Rice University, cflandes@rice.edu*
Stephan Link, *Rice University, slink@rice.edu*

Towards Predictive Calculations in Strongly Correlated Molecules and Materials

From catalysts to chromophores to magnets, many molecules and materials exhibit an electronic structure qualitatively different from the independent-particle physics of Hartree-Fock and density functional theory. Indeed, the mean-field techniques underpinning much of traditional quantum chemistry are notorious for making unreliable predictions in such "strongly correlated" systems. This symposium will emphasize recent work on theoretical models and algorithms that seek to offer affordable predictive power in strongly correlated systems, including novel wave function methods, quantum Monte Carlo, cluster embedding, density matrix reconstructions, and many-body Green's function techniques. In addition to addressing strong correlation in molecules' ground and excited states, the symposium will explore related techniques for nanostructures, solids, and electron transport.

Eric Neuscamman, *University of California-Berkeley, eneuscamman@berkeley.edu*
Timothy C. Berkelbach, *Princeton University, tcb2@princeton.edu*

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session, which will be held on Wednesday evening, 16 March 2016, 6:00 to 8:00 PM. See announcement below for information about the Physical Chemistry Student Poster Awards.

Gregory S. Engel, *University of Chicago, gsengel@uchicago.edu*

On-Line Abstract Submission Deadline: 12 October 2015
http://abstracts.acs.org

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

Six awards with monetary prizes will be awarded for posters presented by students at the Physical Chemistry Poster Session on Wednesday evening of the meeting. 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.

GREGORY S. ENGEL, PROGRAM CHAIR
University of Chicago (773) 834-0818 gsengel@uchicago.edu

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