CALL FOR PAPERS

ACS DIVISION OF PHYSICAL CHEMISTRY
FALL 2020 NATIONAL ACS MEETING

THEME: Moving Chemistry from Bench to Market

16-20 August 2020 San Francisco, California

The ACS Division of Physical Chemistry is hosting the following oral symposia, consisting of both invited and contributed papers, as well as a general poster session.
The abstract submission deadline is 6 April 2020. 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.

Addressing Chemical Complexity with Nonlinear Optical Microscopy

Despite its introduction almost three decades ago, the ability to couple the measurement of nonlinear phenomena with the spatial resolution of a microscope objective has continued to rapidly evolve through both the application of more sophisticated techniques and the study of more complex systems. Progress in the field of nonlinear microscopy has afforded deep penetration in biological tissues, additional modalities for chemical contrast, and dynamics on ultrafast timescales. Challenges remain, however, in extracting new information from increasingly congested samples with minimal perturbation. Innovations in instrumentation, the development of new image analysis methodologies, and novel applications of existing techniques promise new insight into intrinsically heterogeneous samples. This symposium will gather scientists from the fields of chemistry, physics, engineering and biology into a collaborative environment where ideas of technology innovations and sample applications can be shared and discussed. Progress, existing challenges, impact will be emphasized.
Tessa R. Calhoun, University of Tennessee, Knoxville, *trcalhoun@utk.edu*
Martin Fischer, Duke University, *martin.fischer@duke.edu*

Surface-Enhanced Spectroscopy: From Fundamentals to the Marketplace

Mechanisms and exploitation of surface-enhanced spectroscopies span fundamental disciplines in chemistry and physics to more applied areas of applications in biology, engineering, and medicine. This symposium will encompass fundamental research in surface-enhanced spectroscopy including surface-enhanced Raman scattering (SERS), tip-enhanced Raman scattering (TERS), and surface-enhanced hyper-Raman scattering (SEHRS). Key advances for commercial applications such as assay development, big data methods, instrumentation, miniaturization, and substrates will also be covered. This symposium will highlight how fundamental bench and theoretical research on surface-enhanced spectroscopy is being translated into new technological advances. To capture this dynamic area, this symposium will bring together both academic and industrial leaders to share their current work and visions for the future.
John Camden, University of Notre Dame, *John.Camden@nd.edu*
Amanda J. Haes, University of Iowa, *amanda-haes@uiowa.edu*

Single-Molecule Microscopy of Molecular Search Processes: Fundamental Biophysics Inquiry to Pharmaceutical Applications

As microscopy techniques become increasingly sophisticated, researchers are teasing apart the intricacies of biomolecular interactions at the single-molecule level. Of particular interest are the processes of molecular searching, recognition, and binding, as they underpin virtually all critical cellular processes. This symposium will bring together researchers interested in this fascinating out-of-equilibrium problem to study the dynamics of a molecule's search for its target. It will include in vitro and in vivo and imaging methods with single-molecule resolution – such as TIRF, CLiC, curtains, tweezers, super resolution imaging tools as well as theoretical and modeling approaches. Chemists, biophysicists, biologists, as well as pharmaceutical scientists will contribute talks from both applied and fundamental research perspectives. As a group, we will discuss cutting-edge progress in applying advanced techniques to the fundamentally important question of how biomolecules look for, recognize, and bind to their targets. In particular, these insights are valuable to emerging classes of oligonucleotide therapeutics such as antisense oligonucleotide, RNA silencing, and CRISPR systems.
Sabrina Leslie, McGill University, *sabrina.leslie@mcgill.ca*
Corey Nislow, University of British Columbia, *corey.nislow@ubc.ca*

Spectroscopy for Understanding Catalysis

Mechanistic insight into catalysis is a target of some of the most cutting edge tools in optical spectroscopy. These tools span a tremendous array of energies, from meV to keV, are capable of revealing dynamics occurring on timescales ranging from seconds to femtoseconds, and are applied on both large chemical ensembles and single particles and molecules. Taken together, these techniques have revealed the existence of previously unknown chemical intermediates, characterized the structure of transient species, helped to refine chemical pictures of reaction mechanisms, and even informed new cycles of catalyst design. This symposium will bring together physical chemists studying catalysis. Experimentalists covering a wide array of techniques will be included, as will synthetic chemists who will provide useful background information from their complementary perspective and could help identify new problems for the application of spectroscopy. The goal of this symposium is to determine, as a community, places where complementary techniques can amplify mechanistic insights and new opportunities for future spectroscopic explorations.
Randall H. Goldsmith, University of Wisconsin, *rhg@chem.wisc.edu*
Josh Vura-Weis, University of Illinois, *vuraweis@illinois.edu*

Molecular Excitation Induced Dynamics in Chemical & Biological Systems: Celebrating the Achievements of Bradley Moore

C. Bradley Moore is a pioneer of using lasers to induce and probe chemical processes. He was among the first to use lasers to excite specific quantum states of molecules and to probe the ensuing dynamics. He recognized the potential of using IR lasers for selective vibrational excitation and his group performed ground breaking state-to-state energy transfer measurements for many small molecules in gases and in rare-gas matrices. He studied chemically reactive collision partners that permitted reaction rates to be measured as a function of reagent vibrational state and demonstrated how radiationless processes and unimolecular reactions of prototype molecules like formaldehyde and ketene can be studied with state specificity. By elucidating internal conversion, intersystem crossing and collisional quenching, Moore's group produced the first set of quantum-state-resolved unimolecular reaction rates. This symposium will include talks on these topics and provide the community the opportunity to celebrate Moore's lifetime of achievements.
Michael R. Berman, Air Force Office of Scientific Research, *michael.berman@us.af.mil*
Hai-Lung Dai, Temple University, *hai-lung.dai@temple.edu*
Linda Young, University of Chicago, *lindayoung@uchicago.edu*

Advances in Nonlinear Optics at Interfaces

Interfaces are of fundamental importance in catalysis, energy storage and conversion, biological processes, environmental issues, and technological problems such as oil extractions. Understanding the molecular behaviors at interfaces is essential for both basic concepts and industrial applications. In the past decades, powerful nonlinear optical spectroscopy techniques have been developed and applied to reveal behavior of interfacial chemical systems on the molecular level. This symposium will bring together both theoretical and experimental physical chemists who are interested in interfacial chemistry and physics. The proposed speakers include experts in areas ranging from environmental science, biology, to material sciences.
Alex Benderskii, University of Southern California, *alex.benderskii@usc.edu*
Yi Rao, Utah State University, *yi.rao@usu.edu*

Molecular-scale Photoinduced Driving Forces for Energy Conversion

Efficient utilization of sunlight to generate electricity was demonstrated in the 1950s at Bell Labs using crystalline silicon photovoltaics. While photovoltaics are steeped in the history and nomenclature of solid-state physics, chemists have expanded on this initial discovery with the development of new materials and molecule–material hybrids with complex structures on the molecular level, and have also coupled light-absorption processes to bond-making and bond-breaking events. In any of these processes, the charge separation event constitutes photovoltaic action. This symposium aims to capture cutting-edge aspects of photovoltaic action furthered by chemists and chemical engineers and relevant to applications in solar cells and photoelectrochemistry. Attention will be paid to the chemical language, research outcomes, and advanced techniques and computational capabilities utilized in the physics of solar energy conversion, with a specific focus on species transport and charge separation. Species include those that are charged (electrons, ions, polarons, etc.) and neutral (excitons, photons, molecules, etc.), while techniques include those based on spectroscopic, microscopic, electric, electrochemical, and thermal analyses. Experimentalists and theoreticians are expected to contribute to our symposium with research focuses that span all aspects of fundamental science and engineering.
Shane Ardo, University of California, Irvine, *ardo@uci.edu*
Naomi Ginsberg, University of California, Berkeley, *nsginsberg@berkeley.edu*

Structure, Self-Assembly, and Transport in Ionic Systems

Many applications in chemistry, biology, and energy storage/conversion research rely on understanding of fundamental correlations between structural and transport properties in materials with high ionic concentrations. Whether the system is comprised only of ions, e.g. ionic liquids, or is a mixture of a polar solvent or polymers with a salt, e.g. electrolytes for battery applications, the interplay between van der Waals and electrostatic interactions often leads to nanoscale structural heterogeneity, self-assembly and strong dynamic correlations defining ion transport. The understanding of underlying correlations is challenging experimentally and computationally due to their complex and interdisciplinary nature. This symposium will provide a discussion platform for theoretical, modeling and experimental scientists and experts to exchange ideas on developing novel and synergistic characterization and modeling techniques and applications of these methods to advance our understanding of the coupling between structural properties and transport processes in bulk ionic systems and at interfaces. Primary focus will be on the self-assembly, structural heterogeneity, and charge/mass transport in ionic liquids and their mixtures, organic and aqueous electrolytes, polymer and polymer gel electrolytes, polyelectrolyte membranes for applications in batteries, electric double layer capacitors, fuel cells, actuators and electromechanical transducers, and other energy storage/conversion applications.
Paschalis Alexandridis, University at Buffalo, *palexand@buffalo.edu*
Dmitry Bedrov, University of Utah, *d.bedrov@utah.edu*

Biophysical Chemistry in Complex Environments: Convergent Studies of Biomolecular Structure and Dynamics

Biological environments, e.g., the interior of cells, are spatially heterogeneous, crowded, and chemically diverse. The great majority of biophysical studies have been performed using simple buffer solutions, but it is now becoming evident that the environment plays a significant role in determining the structure, dynamics, and folding mechanisms of biomolecules. Recently, many researchers have begun developing methods to investigate biomolecules in "complex" solutions, such as proteins in crowded, cell-like environments, the effect of lipid composition on membrane proteins, or protein structure and dynamics in osmolytes, denaturant, or cryoprotectant mixtures. While these systems remain challenging to investigate, interest has grown in translating experimental techniques, such as time-resolved IR spectroscopy towards systems with increased molecular diversity and spatial heterogeneity. Similarly, enhanced-sampling methods and modern computer resources have enabled large-scale MD simulations that cover multimillion-atom systems over long timescales, which allow for atomistic studies of realistic mimics of cell membranes or even entire portions of the cell cytoplasm. Accordingly, this symposium will bring together experimentalists and theorists who apply cutting-edge methods towards investigating biomolecules in membranes, denaturant solutions, or in crowded environments.
Carlos Baiz, University of Texas, *cbaiz@cm.utexas.edu*
Angel E. Garcia, Los Alamos National Labs, *agarcia@lanl.gov*

Atomistic Characterization of Electrochemical Interfaces

The interface formed between an electrode and electrolyte is the ultimate playground for physical chemists. These interfaces host a multitude of coupled physical and chemical processes, including redox reactions, electron transport, phase transitions, and ion-ion interactions, all of which are further complicated by the heterogeneous nature of the interface. Furthermore, applied voltage (or photons in light-sensitized systems) can be used as a knob to turn up the dial on these processes. The physical chemistry is thus rich and highly complex, and qualitatively altered through external modulation. Fundamental understanding and atomistic insight require the combination of modern state-of-the-art spectroscopy and imaging techniques, and ab initio modeling and computer simulations. This symposium will bring together both experimental and theoretical/computational researchers to discuss recent discoveries and developments in the atomic-level understanding of electrochemical interfaces. Topics will include electrochemical energy storage, electro-catalysis applications, and other topics. The focus will be on atomistic/microscopic characterization of these interfaces, with an emphasis on developing detailed structural, dynamical, and mechanistic understanding. The purpose of the symposium is to both stimulate and disseminate novel research directions in the field, as well as to discuss and improve the bridging of experimental and theoretical characterization of these systems.
Oleg Borodin, Army Research Laboratory, *oleg.a.bordin.civ@mail.mil*
Jesse McDaniel, Georgia Tech, *mcdaniel@gatech.edu*
Yue Qi, Michigan State University, *yueqi@egr.msu.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/postdocs/announce_2020.html

Physical Chemistry Poster Session

Contributions from all areas of physical chemistry are highly encouraged for the poster session (likely on Wednesday from 6:00 to 8:00 PM, but check schedule). Up to six 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: 6 April 2020
http://abstracts.acs.org

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