ACS DIVISION OF PHYSICAL CHEMISTRY
253RD NATIONAL MEETING

***THEME:* Advanced Materials Technologies, Systems and Processes**

2-6 April 2017 ◆ San Francisco, 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 September 5th. **The abstract deadline is 31 October 2016**. 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.

Dynamics and Structure of Molecular Fluids: A Symposium in Honor of Branka Ladanyi

When the general public thinks of chemistry, they envision reactions occurring in beakers and flasks filled with liquid solutions. Chemistry often focuses on the solutes in these chemical systems—but what of the fluids that support those reactions? This symposium will present results from the wide-ranging studies (both theoretical and experimental) exploring the structure and dynamics of fluids, including bulk liquids, liquids in confined environments, microemulsions, supercritical fluids and molecular clusters. This symposium will highlight studies that aim to unravel the complex dynamics in these systems and phenomena at a microscopic level—a goal that has challenged scientists for generations and one that is critical for the comprehension of real chemical processes. These systems formed the basis of the far-reaching and significant contributions from the late Prof. Branka Ladanyi, whose scientific contributions added profoundly to the theory and modeling of molecular fluids, and stimulated significant collaborations between theorists and experimentalists. This symposium will feature invited and contributed talks in honor and memory of Branka.

Nancy E. Levinger, Colorado State University, *Nancy.Levinger@colostate.edu*
Amber Krummel, Colorado State University, *Amber.Krummel@colostate.edu*

Spectroscopy of Complex Systems

A diverse array of modern spectroscopies, in particular ultrafast time-resolved and nonlinear optical techniques, have been developed for probing complex chemical and biological systems. These methods provide a wealth of information on the molecular structure and dynamics of complex and unconventional environments, from bulk liquids and interfaces to nanostructures and proteins. Despite the wide range of techniques and applications, there are common physical and chemical question underlying the microscopic behavior of these systems. These are fundamental to our understanding of chemical properties and ability to predict them. This symposium brings together researchers from different areas of modern spectroscopy to facilitate discussions emphasizing the unifying physical/chemical principles. The sessions are organized accordingly, with the talks grouped by the common fundamental questions that are manifested in different types of molecular systems and are studied by different spectroscopic techniques. These include: the role of asymmetry, nanoconfinement, and local electric fields on molecular dynamics in heterogeneous environments such as interfaces, electrode surfaces, plasmonic structures, and proteins, proton and electron transfer in biological systems, and exciton dynamics in homogeneous and heterogeneous systems.

The symposium stresses the importance of theory in the interpretation of modern spectroscopic measurements and the design of new experiments by bringing together experimentalists and theorists working on systems and techniques that do not normally overlap in order to facilitate new interactions and collaborations.

Alex Benderskii, University of Southern California, alex.benderskii@usc.edu
Jahan Dawlaty, University of Southern California, dawlaty@usc.edu

Expanding the Frontiers in Condensed Phase Astrochemistry: Electron Transfer Processes in Ices and Catalysis on Interstellar Grains

Significant new experimental techniques have been developed during the last decade to investigate the interaction of ionizing radiation and of neutral atomic and molecular species with surface analogs of solids in the Solar System and in the Interstellar Medium (ISM). Investigation of these chemical processes provide fundamental insight at the molecular level into the chemical evolution of the interstellar medium, planet forming regions, and on/in icy objects in the Solar System. The chemical complexity covers a wide range from the formation of the simplest molecule (molecular hydrogen) to complex biomolecules such as amino acids and sugars. Two ongoing space missions to the Kuiper Belt (New Horizons) and comet 67P/Churyumov–Gerasimenko (Rosetta) highlight the importance of understanding these processes. This symposium features invited and contributed talks on experimental and computational work covering the interaction of ionizing radiation (UV, VUV, gamma rays, charged particles) and neutrals (atoms, radicals, molecules, grains) with low temperature solids (ices, minerals, organics) towards the formation of solids (complex organics, interstellar grains, nanoparticles) from simple silicon- and carbon-bearing precursors.

Ralf I. Kaiser, University of Hawaii, *ralfk@hawaii.edu*
Murthy S. Gudipati, NASA Jet Propulsion Laboratory, *Murthy.Gudipati@jpl.nasa.gov*

Multicenter Molecules and Coupled Molecular Assemblies: Synthesis, Characterization, and Theory

The theme of this symposium is the design and characterization of systems of interacting multicenter molecules (i.e. molecules that support multiple stable electronic configurations). A classic example of a multicenter molecule is a mixed valence compound that contains a pair of metal sites that can change their oxidation state through electron transfer. Coupled molecular systems represent a new paradigm for information transfer and processing at the ultimate limits of the length scale—the single molecule. The charge distribution of a multicenter molecule is strongly coupled to that of neighboring molecules. This property can be exploited to create controlled interactions between molecules, potentially forming large-scale assemblies that store information or perform computation. Moreover, new approaches to bridging the macroscopic and molecular length scales, which is a major challenge in applying nanotechnology into practical devices, can result by interfacing coupled molecular assemblies with external electric fields. This symposium will bring together researchers in synthesis, physical characterization, and theory to foster discussion of new paradigms for utilizing multicenter molecules and coupled molecular assemblies toward new technology.

Steven A. Corcelli, University of Notre Dame, *steven.a.corcelli.1@nd.edu*
Kenneth W. Henderson, Northeastern University, *k.henderson@northeastern.edu*

Sunlight-driven Processes: Exposing the Mechanisms Underlying Productive Photoactivities

The proposed symposium offers an uncommon wide view of recent developments in the molecular-lever and electronic-level understanding of (sun)light-driven processes from biological systems to material design. Light-induced processes fundamentally rely on using coupled electronic and nuclear motions enabled by photon absorption. Whether photoisomerisation, proton or electron-transfer, all cases are driven by the initial absorbed photon energy which is then transduced into electronic and vibrational dynamics. Thus, the design and synthesis of molecules or molecular complexes that efficiently exploit light to drive wanted functions, must necessarily relay on the intimate knowledge of the mechanisms that efficiently converts the absorbed energy into specific electrons or atomic motions. The main target of the symposium is to provide an opportunity to discuss interdisciplinary and complementary research efforts for exploring the mechanisms underlying the exploitation of sunlight going from biological to engineering materials. Emphasis will be given to the understanding of the electronic, atomic and molecular details of these processes "resolved' via complementary experimental and computational approaches. The hope is to highlight how, presently, the mechanistic understanding of biological light-driven functions are, or might be, exploited in the development of functional materials going from light energy harvesting and storing materials to photocatalytic materials.

Massimo Olivucci, Bowling Green State University, *molivuc@bgsu.edu*
Delmar S. Larsen, UC Davis, *dlarsen@ucdavis.edu*
Ksenija D. Glusac, Bowling Green State University, *kglusac@bgsu.edu*

Plasmonic Nanomaterials: From Physical Chemistry Fundamentals To Societal Impacts

The National Nanotechnology Initiative began in 2001 in the U.S., catalyzing an enormous burst of research activity in the area of nanomaterials. The promise of the investment was predicated on new materials and applications that could not only stimulate science but also stimulate innovation, technology, and societal good in the form of the economy. A good question to ask in 2017 is: How far have we come? How well do we understand the fundamentals of nanomaterials, and how much of our knowledge has led to new technologies? Because the field of nanomaterials is so broad, this symposium will focus on plasmonic nanomaterials. The particular topics include metamaterials and information technology; surface chemistry, sensors, and diagnostics; plasmonic solutions to the energy problem; plasmonic solutions for medicine. We aim to have at least one industrial speaker/entrepreneurial professor per session who can speak to the societal impact of the science and technology.

Catherine J. Murphy, University of Illinois at Urbana-Champaign, *murphycj@illinois.edu*
Prashant K. Jain, University of Illinois at Urbana-Champaign, *jain@illinois.edu*

Quantum Dynamics in Large Scale Systems

This symposium will bring together leading experts and young researchers who develop new approaches to quantum dynamics and quantum chemistry in extended systems. A broad range of topics focusing on fundamental challenges, as well as methodological and practical aspects of large-scale calculations in quantum dynamics will be discussed.

The symposium will foster merging the two presently distant worlds: the field of stationary quantum calculations in large-scale systems and the field of atomistic simulations of quantum dynamical processes. The symposium will aim to discuss the existing techniques for above calculations - their capabilities and limitations, as well as the challenges researches face or will be facing in the near future. A special interest will be to discuss the challenges that arise when the two worlds meet each other.

The main focus will be on the methodological and theoretical advances, but the discussion of the studies of large atomistic systems representing modern materials will be undertaken. Application-wise, we will be interested to discuss studies in the systems that are hard to model using conventional methods: large quantum dots, nanoscale structures, interfacial and polymeric systems. We will also discuss fundamental aspects needed for successful integration of the stationary and dynamical approaches.

Oleg V. Prezhdo, University of Southern California, *prezhdo@usc.edu*
Alexey V. Akimov, University at Buffalo, a*lexeyak@buffalo.edu*

Long-range Correlated Motions in Proteins

This symposium will explore different experimental and computational techniques to understand the role of long-range correlation motions in biomolecular function. Invited speakers from a variety of experimental fields and computational approaches will specifically consider how long range structural dynamics can influence allosteric control. We will also focus on key issues for understanding structural dynamics, namely proper modeling of the solvent, and measurements of protein crystals. Over the last several years a number of groups have demonstrated that intramolecular long range correlated motions can be observed, however the effect of the intermolecular bonding on these dynamics is not well characterized. Modeling of these constraints is also an area of intense study. The invited speakers list come from a broad spectrum of fields, institutions and approaches. We expect the symposium will provide a lively forum for the understanding and further development of protein dynamics studies.

Andrea Markelz, SUNY Buffalo, *amarkelz@buffalo.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, 5 APRIL 2017, 6:00 to 8:00 PM. See announcement below for information about the Physical Chemistry Student Poster Awards.

Joan-Emma Shea, University of California, Santa Barbara, *shea@chem.ucsb.edu*

On-Line Abstract Submission Deadline: 31 October 2016
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.

JOAN-EMMA SHEA, PROGRAM CHAIR
University of California, Santa Barbara, Department of Chemistry and Biochemistry (805) 893-5604 shea@chem.ucsb.edu

FOR INFORMATION ABOUT THE PHYSICAL CHEMISTRY DIVISION, VISIT OUR WEB SITE: http://phys-acs.org/