ACS DIVISION OF PHYSICAL CHEMISTRY
243rd NATIONAL MEETING
San Diego, CA
March 25-29, 2012

Call for Papers

The Physical Chemistry Division has organized the following topical oral symposia, consisting of both invited and contributed papers, and also topical and general poster sessions. **The abstract deadline is October 17, 2011**. 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 presentation; contributions not selected for oral presentation will be assigned to the poster session.

WATER MEDIATED CHEMICAL ASSEMBLY

This symposium focuses on experimental, theoretical, and simulation studies of water's active role in mediating and driving the structure and dynamics of systems including hydrated molecules, clusters, nano-particles, biopolymers, and interfaces. Although pure water and simple aqueous solutions have been extensively studied, vast structural regimes and dynamical landscapes associated with water's role in biological and nano-material chemical-assembly remain to be explored. These include elucidating the impact of cooperative (non-additive/synergetic) phenomena in materials ranging from hydrated molecular clusters (at low temperature in the gas phase) to aqueous solutions and nanometer aggregates (at room temperature in the liquid phase), as well as understanding the changes in water's structure and dynamics as it interacts with small molecules, nano-particles, and macroscopic objects. Moreover, collective motions of water networks spanning time scales ranging from femtoseconds to hours hold a wealth of information about how water molecules facilitate and drive chemical assembly in systems ranging from biological proteins to nano-composites. This symposium provides a forum for reporting and discussing emerging experimental and theoretical developments in these forefront areas, as well as promoting the innovation of water-mediated nano-machines, devices, and materials.

Dor Ben-Amotz, *Purdue University, bendor@purdue.edu*
Dmitry Matyushov, *Arizona State University, dmitrym@asu.edu*

SINGLE MOLECULES: THEORY MEETS EXPERIMENT

Advances in single molecule manipulation and detection have found wide applications at the interface of chemistry, physics, and biology. The single-molecule approach allows us to observe transient states and kinetic pathways that are difficult to resolve in ensemble measurements, thus providing insights that stimulate new theories and models. Indeed, the field of single molecules has benefited greatly from the lively interactions between theory and experiment, which will be highlighted in this symposium. The proposed symposium features a mixture of physical chemists and biological chemists, and includes a diverse range of subsections: (1) single molecule methods, (2) conformational dynamics, (3) nano/exciton systems, (4) biological applications, (5) photo-synthetic systems, and (6) bio-mechanics.

Robert Dickson, *Georgia Institute of Technology, robert.dickson@chemistry.gatech.edu*
Jianshu Cao, *Massachusetts Institute of Technology, jianshu@mit.edu*

FROM GEOCHEMISTRY TO BIOCHEMISTRY AND THE ORIGIN OF LIFE

Planetary chemistry set the stage for the emergence of biochemistry from geochemistry. Physical conditions on ancient Earth gave rise to abiotic organic synthesis, which generated a heterogeneous mixture of small molecules and polymers. Entropically driven organization of the available abiotic molecular species resulted in the emergence of molecular systems capable of metabolism, self-replication, and evolution. Interactions between the atmosphere, ocean, mineral surfaces, and space impacted all of these processes, ultimately generating micro- and macroscopic systems. This symposium proposes to bring together chemists working on atmospheres and oceans, on chemical evolution and on biophysical processes necessary for the synthesis of model protocells. On ancient Earth, the air-ocean interface would have acted as a two-dimensional concentrator and integrator of three-dimensional chemistry in the atmosphere and the ocean. Chemical processes would have been shaped by meteoritic infall, hydrothermal vents on the sea floor, icy particles in the atmosphere, and minerals on the Earth's surface, eventually leading to biomolecular synthesis. The symposium will highlight studies from diverse chemical communities contributing to the understanding of key molecular processes fundamental to life.

Veronica Vaida, *University of Colorado, vaida@colorado.edu*
Sheref Mansy, *Universita di Trento, sherefsamir.mansy@unitn.it*
Ulrich Muller, *University of California San Diego, ufmuller@ucsd.edu*

FRONTIERS IN HETEROGENEOUS CATALYSIS

Recent experimental and theoretical advances present us with the opportunity to describe and control catalytic systems at an atomic level. Presentations leading to the understanding of fundamental principles and structure-reactivity relationships will form a focal point of this symposium. The emphasis will be put on a synergistic approach between theory and experiments. Sessions dealing with model metal and metal-oxide catalytic systems, nanoscale induced reactivity, structure-reactivity relationships, and non-thermal processes will be held to stimulate the exchange of ideas and the formation of new collaborations in this interdisciplinary field.

Roger Rousseau, *Pacific Northwest Laboratory, roger.rousseau@pnl.gov*
Zdenek Dohnalek, *Pacific Northwest Laboratory, zdenek.dohnalek@pnl.gov*

NONADIABATIC DYNAMICS: SURFACE HOPPING AND BEYOND

Surface hopping, pioneered by Tully and Preston in 1971, represents the most popular family of non-adiabatic molecular dynamics (NAMD) techniques. NAMD has become a major approach for modeling chemical events that involve transitions between multiple quantum states. Surface hopping treats the transitions as stochastic events, in the spirit of the probabilistic interpretation of quantum mechanics. Examples of such studies abound, ranging from scattering of atoms and small molecules in gas phase, to photoinduced reactions in condensed phases, including solutions, polymers, inorganic materials and organic-inorganic interfaces, to biological processes such as photosynthesis and vision. The surface hopping simulations are strongly motivated by time-resolved optical experiments that are carried out by multiple research groups in every major research university. Some of the recent applications of NAMD include solar energy harvesting, inelastic processes in molecular electronics, biological optical probes, light emitting diodes, laser control of chemical reactivity and quantum information processing. The symposium aims for a timely discussion of modern developments, applications and challenges in surface hopping, nonadiabatic molecular dynamics and quantum dynamics in general.

Oleg Prezhdo, *University of Rochester, prezhdo@chem.rochester.edu*
Xiaosong Li, *University of Washington, li@chem.washington.edu*

CURRENT VIEWS ON SECONDARY STRUCTURE

Since Pauling's 1948 proposal of the alpha helix and beta sheet conformations of the polypeptide backbone, secondary structure has been a central element in the description of protein structure, thermodynamics, and folding. Advances in experimental and computational techniques, the development of robust model systems, and the convergence of experimentally and computational accessible time scales have combined to produce detailed pictures of the thermodynamics and kinetics of the formation of secondary structure in proteins. This symposium addresses contemporary experimental and theoretical efforts towards the understanding of secondary structure, including analysis of helix and hairpin stability; kinetics and mechanistic studies of helix and beta hairpin formation; the effects of membranes, micelles, and solvent environment on polypeptide backbone conformation; and the nature of random coil and polypeptide states.

Angel Garcia, *Rensellaer Polytechnic Institute, angel@rpi.edu*
Feng Gai, *University of Pennsylvania, gai@sas.upenn.edu*
Sean Decatur, *Oberlin College, sean.decatur@oberlin.edu*

PHYSICAL CHEMISTRY OF CO_2 SEPARATION

Managing the impact of human activities on the amount of CO_2 in the atmosphere is the most far-reaching environmental challenge facing the world today. Our highly developed fossil fuel infrastructure, the relative inexpensiveness and convenience of this natural resource, and current estimations that these fuel reserves will last for at least several more centuries only bolster the proposition that fossil fuels will continue to dominate the energy landscape for the foreseeable future. And even as society adopts renewable sources of energy such as solar and wind, it is quite likely that at least a portion of the harnessed energy will be used to convert captured CO_2 into hydrocarbon fuels. Any strategy for managing the CO_2 problem involves at some stage taking CO_2 from a relatively dilute source—a flue gas, a natural gas stream, even the atmosphere—to a high purity state suitable for usage or storage. This symposium will focus on the science of these CO_2 separations, from the design and development of novel CO_2 separating materials, to their molecular characterization and simulation, to considerations relevant to their real-world application. The symposium will provide a forum for exchange amongst leaders in the field and an opportunity for the Physical Chemistry community to be introduced to the key scientific challenges and opportunities.

William Schneider, *University of Notre Dame, wschneider@nd.edu*
Abhoyjit Bhown, *Electric Power Research Institute, abhown@epri.com*

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday evening, March 28, 2012. See announcement below for information about the Physical Chemistry Student Poster Awards.

Martin Gruebele, *University of Illinois, mgruebel@illinois.edu*

We welcome suggestions for future symposia!
Please send your ideas to the 2013 Program Chair,
Joel Bowman, Department of Chemistry,
Emory University, Atlanta, GA 30322, (404) 727-6592,
jmbowma@emory.edu

On-Line Abstract Submission Deadline:
October 17, 2011
http://abstracts.acs.org

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

At the meeting in San Diego, CA, several 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.

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