



ACS DIVISION OF PHYSICAL CHEMISTRY
240th NATIONAL MEETING
BOSTON, MA
AUGUST 22-26, 2010



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 April 5, 2010.** 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.

ELECTRONS IN BIO-MOLECULES

Electron attachment and transfer and electronic excitation play important roles in many aspects of the chemistry of biologically relevant molecules. The behavior of biomolecules upon electronic excitation and electron attachment and transfer is relevant to both functionality (e.g. photosynthesis) and damage mechanisms (e.g. through formation of radicals). To name just a few examples: In analytical mass spectrometry, electron capture and subsequent dissociation is used as a powerful structural probe. Electronic spectroscopy techniques are key to the elucidation of structures, energetics and dynamics of biomolecules. Electron attachment to DNA has been shown to be at the heart of a variety of processes relevant to DNA damage by ionizing radiation. This symposium is meant to bring together experimental and theoretical chemists who are studying the structures of biomolecular anions, how electrons are attached to or promoted to excited states in biomolecules, and how attached or excited electrons induce bond cleavages in biomolecules.

Jack P. Simons, *University of Utah*, jack.simons@utah.edu

J. Mathias Weber, *University of Colorado*, weberjm@jila.colorado.edu

MOLECULAR SYSTEMS FOR EFFICIENT SOLAR ENERGY CONVERSION AND STORAGE

Molecular systems for efficient solar energy conversion and storage have attracted a great deal of attention in the Physical Chemistry and Physico-Inorganic Chemistry communities. Photoconversion mechanisms triggered by the interaction of light with novel, chemically designed materials are investigated from the point of view of fundamental science and in the quest for chemical principles to guide the rational design of efficient photovoltaic and photocatalytic systems. This symposium aims to survey recent advances in studies of new materials, electronic processes, and reaction mechanisms for solar energy harvesting and conversion into electrical and chemical forms. The program is intended to bring together a diverse community to foster the cross-fertilization of complementary approaches in the development and characterization of molecular systems for efficient and cost effective solar energy conversion.

Victor Batista, *Yale University*, victor.batista@yale.edu

Charles Schmuttenmaer, *Yale University*, charles.schmuttenmaer@yale.edu

Gary Brudvig, *Yale University*, gary.brudvig@yale.edu

CHALLENGES FOR DENSITY FUNCTIONAL THEORY

As density functional theory (DFT) has become a main tool of modern computational applications and simulations, it also faces major challenges from many areas of research. Many critical failures have been observed, and recently, major progress has been made in understanding and addressing these failures. In this symposium, we plan to focus on two broad topics including ground-state and time-dependent DFT. The former is the most widely used form of DFT. Although commonly used approximate functionals underlie the success of many computational studies using DFT, they are also responsible for the failures. On the other hand, in the time-dependent domain, due to the lack of non-adiabatic exchange-correlation kernels, TDDFT work mostly remains in the perturbative regime within the adiabatic approximation. Although a number of numerical methods have been developed to model real-time electronic dynamics, they can only provide a qualitative description of electronic systems beyond the ground state. This symposium aims for a timely discussion on DFT developments and applications that will bring up extensive discussions on challenges for DFT.

Weitao Yang, *Duke University*, weitao.yang@duke.edu

Xiaosong Li, *University of Washington*, li@chem.washington.edu

PHYSICAL CHEMISTRY OF SPECTROCHEMICAL ANALYSIS

Physical chemistry has long played a role in translating new technologies for spectroscopy into tools for chemical analysis. Technological advances with potential impact for spectroscopy can come from a variety of areas including new device technology, advances in light sources, and the discovery of new physical effects that enhance sensitivity. This symposium will highlight instrument development programs in physical chemistry that are bringing new technology into the field of spectrochemical analysis. These advances include new coherent light sources for broadband spectroscopy and ultrafast spectroscopy, the exploitation of structured nanoscale materials for high-sensitivity detection, and the emergence of high-speed digital electronics that provide the data throughput rates needed to transform spectrometers into real-time chemical sensors. The convergence of these technologies into chemical imaging systems that combine high-spatial resolution with broadband spectroscopic detection is a theme that will be explored.

Brooks H. Pate, *University of Virginia*, brookspate@virginia.edu

Kevin K. Lehmann, *University of Virginia*, kl6c@virginia.edu

METALS IN BIOLOGY

Transition metals play an essential role in metabolic processes throughout the three kingdoms of life and thus are critical to life as we know it. One third of all proteins contain metal ions as cofactors and these metals serve a plethora of functions including stabilization of tertiary structure, facilitation of the transfer of electrons, as well as binding and activation of small molecules and metabolites.

This symposium will highlight the rich diversity of metal active sites and the reactions they catalyze, emphasizing connections between inorganic chemistry, mechanistic enzymology, spectroscopy, and structural biology. The symposium will also emphasize emerging themes in transition metal metabolism and cellular homeostasis, including areas such as metal acquisition, availability, and export; and fluorescent tools for imaging metal distribution and mobilization in cells.

Amy Palmer, *University of Colorado*, amy.palmer@colorado.edu

Thomas Brunold, *University of Wisconsin*, brunold@chem.wisc.edu

PHYSICAL CHEMISTRY SYMPOSIUM WORKSHOP FOR UNDERGRADUATE CHEMISTRY MAJORS

The Workshop for Undergraduate Chemistry Majors is targeted for current junior chemistry majors, who will be seniors at the time of the Boston meeting. Up to 25 outstanding undergraduate chemistry students will be selected for a series of undergraduate-focused talks and social events during the Boston meeting. In addition, they will be expected to present posters on their research as part of the PHYS poster session. More information and application materials can be found at <http://www.phys-acs.org/UGworkshop10.html>. The application deadline is February 12, 2010.

William Polik, *Hope College*, polik@hope.edu

PHYSICAL CHEMISTRY OF HYDRATES, INTERFACES AND AEROSOLS AND THEIR RELATIONSHIP TO CLIMATE

The drivers of radiative forcing in the Earth's atmosphere are greenhouse gases and aerosols, both of which undergo chemical transformations that affect their optical properties, lifetimes, distributions and long-term trends. Recent theoretical, laboratory and field studies have identified key uncertainties and advanced the fundamental understanding of such processes. These studies have both improved the predictive capability of atmospheric models and demonstrated some of their limitations. This symposium is intended to provide a forum for a subset of current issues at the crossroads between physical chemistry and the climate system.

Water in all its phases, complexes of water and water/ice - air interfaces are of utmost importance in thermostating the atmosphere. The spectroscopy of water vapor and of neutral, ionic and radical water complexes is important in the acquisition of a fundamental spectroscopic and chemical data-base relevant to atmospheric conditions. Water and ice surfaces have recently been shown to be a special chemical environment. Theoretical and experimental methods are being developed to differentiate properties of interfaces from the bulk and provide the molecular information needed to develop predictive models.

Heterogeneous reactions influence the oxidizing capacity of the atmosphere affecting the lifetime of short-lived greenhouse gases such as methane and the distribution of oxidants such as ozone and OH, but are challenging to accurately characterize for realistic atmospheric systems. Atmospheric aerosols influence climate both directly and indirectly. A large fraction of aerosol mass is secondary in nature, occurring through chemical transformations taking place within the atmosphere, yet these transformations remain poorly understood. This symposium seeks presentations aimed at mechanistic elucidation of these and other physical and chemical processes that influence climate.

Veronica Vaida, *University of Colorado*, vaida@colorado.edu

Steven S. Brown, *NOAA*, steven.s.brown@noaa.gov

RECENT ADVANCES IN ION MOBILITY FOR ANALYSIS AND CHARACTERIZATION OF MACROMOLECULES

Ion Mobility is becoming a main stream tool in structural analysis of macro-molecular systems. This is especially true when coupled with Mass Spectrometry (IMS-MS) and high level molecular modeling. Biological systems are being specifically targeted because of the strong structure/function relationship there and because traditional structural methods are often not effective for many important systems. These include, but are not limited to, non-covalent complexes (the primary way most bio-molecules perform their function), aggregating systems (the mechanistic heart of many important diseases, like Alzheimer's, Parkinson's, Diabetes type 2, mad cow, etc), drug-receptor interactions, various "omics" applications like proteomics, glycomics, and imaging of biological tissue. Commercial instrumentation is finally available (Waters Synapt) and more is on the way and new developments promise ever higher resolution and sensitivity. It is the new analytical technique of choice with its roots and continued development firmly planted in the Physical Chemistry community. The time is right for an ACS symposium highlighting the current state of affairs and the directions for the future.

Michael T. Bowers, *U. C. Santa Barbara*, bowers@chem.ucsb.edu

Erin Baker, *PNNL*, erin.baker@pnl.gov

CHEMICAL COMPUTATIONS ON GENERAL PURPOSE GRAPHICS PROCESSING UNITS (GP-GPUS)

Although exact solution of the equations of quantum and classical mechanics is not possible, substantial progress has been made over the past two decades in the solution of these equations using advanced computing technologies. It is now possible to compute many properties of small molecular systems with an accuracy that rivals that obtained in laboratory measurements, and, for larger molecular systems, computations can provide insights into the details of molecular processes that cannot be obtained from experiment alone. As computing technologies continue to advance, significant progress is possible toward many long sought goals in chemistry, e.g., from a deep understanding of the factors that determine the structure, energetics, and dynamics of molecules to the rational design of chemicals, materials, and drugs.

But, computing technologies are changing—processors based on a single core are being left behind, replaced by multi-core and many-core processors. The impact of these technological changes must be understood in order to take full advantage of the opportunities that they offer. One of the most remarkable of these advances has been the development of the General Purpose Graphics Processing Unit (GP-GPU), which uses hundreds of simplified compute cores to achieve speeds well beyond that available with conventional CPUs. A number of chemistry applications have now been implemented on GP-GPUs, achieving speed-ups of one to two orders of magnitude.

This symposium will provide technical presentations from the companies who are advancing the development of GP-GPUs, discussions of the challenges involved in effectively programming GP-GPUs, and presentations on the use of GP-GPUs in a broad range of chemical applications.

Thom H. Dunning, Jr., *University of Illinois*, tdunning@ncsa.uiuc.edu

Volodymyr Kindratenko, *University of Illinois*, kindr@ncsa.illinois.edu

Todd J. Martinez, *Stanford University*, tjm@spawn.scs.uiuc.edu

Robert J. Harrison, *Oak Ridge National Laboratory*, harrisonrj@ornl.gov

Jeffrey Madura, *Duquesne University*, madura@duq.edu

POSTDOCTORAL RESEARCH AWARDS

The PHYS Division plans to highlight leading research by postdoctoral fellows at the Fall National ACS meeting in Boston, through a series of special awards. Awardees will give oral presentations in a PHYS symposium, and attend the PHYS executive dinner. Each postdoctoral nominee should also submit the usual contributed abstract to the PHYS program when on-line submission opens on January 25, so he/she can present at the meeting even if not selected for the special symposium. The deadline for applications is March 10, 2010 and selections will be announced shortly after the Spring ACS meeting in March 2010. More details on the award and applications procedure may be found at <http://phys-acs.org>.

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday evening, August 25, 2010. See announcement below for information about the Physical Chemistry Student Poster Awards.

Mark A. Johnson, *Yale University*, mark.johnson@yale.edu

On-Line Abstract Submission Deadline:

April 5, 2010

<http://abstracts.acs.org>

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

At the meeting in Boston, several awards with monetary prizes will be given 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. Poster presenters will be contacted by e-mail and invited to declare their eligibility (student status) and desire to participate in the student poster award competition.

MARK A. JOHNSON, PROGRAM CHAIR

YALE UNIVERSITY, (203) 436-4930; FAX (203) 432-6144; mark.johnson@yale.edu

FOR INFORMATION ABOUT THE PHYSICAL CHEMISTRY DIVISION, VISIT OUR WEB SITE:

<http://phys-acs.org/>