ACS DIVISION OF PHYSICAL CHEMISTRY
242nd NATIONAL MEETING
DENVER, COLORADO
AUGUST 28- SEPTEMBER 1, 2011

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 March 21, 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.

FROM ULTRAFAST ELECTRON TRANSFER TO SINGLE MOLECULE SPECTROSCOPY: FORCES DRIVING CONTEMPORARY THEMES IN PHYSICAL CHEMISTRY

Physical chemistry is pushing the frontiers of chemical reactivity from ultrafast electron motion during chemical reactions, to pinpointing the chemistry of single molecules. Paul Barbara's legacy exemplifies how chemical problems can be solved with state-of-the-art instrumentation. This symposium looks to the future of ultrafast electron transfer, single molecule spectroscopy, and the physical chemistry of organic-based materials.

Gilbert C. Walker, *University of Toronto, gilbert.walker@utoronto.ca*
Stephan Link, *Rice University, slink@rice.edu*
Christy Landes, *Rice University, cflandes@rice.edu*

HETEROGENEOUS ATMOSPHERIC CHEMISTRY

Chemistry plays a critical role in atmospheric science, from understanding global climate change to regional air quality. This symposium focuses on the current understanding of fundamental physical chemistry processes of the condensed phase components of the Earth's lower atmosphere, atmospheric aerosols, and their surfaces. The symposium highlights the interdisciplinary nature of heterogeneous atmospheric chemistry, with research areas encompassing laboratory study, field observation, and theory. Fundamental aspects of interfacial organization, surface reactions, competitive surface residence, and nucleation will be emphasized. Contributions from a variety of tangential fields infuse new ideas from the frontier areas of physical and atmospheric chemistry to further understand the complexities of heterogeneous atmospheric chemistry.

Heather C. Allen, *The Ohio State University, allen@chemistry.ohio-state.edu*
Martina Roeselova, *Academy of Sciences of the Czech Republic, roesel@uochb.cas.cz*

PUSHING THE ENVELOPE: COMPUTATIONAL CHEMISTRY AT THE PETASCALE AND BEYOND

Computational chemistry has reached the point at which very high quality calculations on complex molecules, such as materials, solid catalysts, proteins, enzymes, and liquids, are becoming feasible. In order to make such calculations a reality on petascale and beyond computing resources, the development of novel software approaches is essential. New, relevant developments include linear scaling algorithms for the most demanding methods, fragmentation approaches that subdivide complex species into smaller, more tractable pieces while retaining high accuracy, multi-level parallelism, grid computing, accelerator algorithms, and novel middleware that sits between the application and the compiler. All of these areas and the challenges toward even higher scaling will be represented in the symposium.

Theresa L. Windus, *Iowa State University and Ames Laboratory, twindus@iastate.edu*
Mark S. Gordon, *Iowa State University & Ames Lab., mark@si.msg.chem.iastate.edu*

ADVANCES IN SERS AND MOLECULAR PLASMONICS

Molecular plasmonics is an emerging field that exploits the interactions of molecules with collective electronic excitations (plasmons) in noble metal films and nanoparticles. The rapidly growing interest in plasmonics stems from the ability to control, manipulate, and amplify light on the nanoscale. This approach has many potential applications, including nanoscale optical spectroscopy, surface-enhanced Raman scattering (SERS), and surface plasmon resonance sensing. This symposium will highlight recent experimental and theoretical advances in the field of SERS and molecular plasmonics.

Lasse Jensen, *Pennsylvania State University, jensen@chem.psu.edu*
Richard P. Van Duyne, *Northwestern University, vanduyne@northwestern.edu*

SYMPOSIUM IN HONOR OF 100TH ANNIVERSARY OF MARIE CURIE'S NOBEL PRIZE FOR INTERNATIONAL YEAR OF CHEMISTRY

This symposium will be a celebration of the current research in physical chemistry conducted by women scientists. The speakers will represent the diverse nature of physical chemistry. The sessions will cover experimental and theoretical research on topics such as surfaces and interfaces, polymers and macromolecules, gas phase ions and clusters, energy and the environment, and biophysics. For more information, go to http://coach.uoregon.edu and click on the "Go Physical" button.

Geri Richmond, *University of Oregon, richmond@uoregon.edu*
Ellen Stechel, *Sandia National Laboratories, ebstech@sandia.gov*
Jeanne M. Robinson, *Los Alamos National Laboratory, jeanne.robinson@lanl.gov*

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 31, 2011. See announcement below for information about the Physical Chemistry Student Poster Awards.

Sharon Hammes-Schiffer, *Pennsylvania State University, shs@chem.psu.edu*

EXCITED STATE DYNAMICS: THEORY AND EXPERIMENT

This symposium will explore experimental and computational efforts to elucidate the dynamics of small molecules, clusters, nanoparticles, and macromolecular systems in excited electronic states, in both gaseous and condensed phase environments. Recent advances in quantum chemistry have enhanced our ability to calculate electronic excitation energies and electronic couplings in large molecules, and to perform excited-state molecular dynamics simulations. At the same time, developments in both time- and frequency-domain spectroscopies continue to push the envelope of what is accessible experimentally, revealing new aspects of molecular photochemistry and photophysics. This symposium will report new experimental results for theorists to rationalize, as well as new theoretical predictions to be tested experimentally, on topics that include nonadiabatic dynamics, photochemistry, ab initio molecular dynamics, excitation energy transfer, and exciton dynamics.

John M. Herbert, *The Ohio State University, herbert@chemistry.ohio-state.edu*
Stephen Bradforth, *University of Southern California, stephen.bradforth@usc.edu*

ADVANCED MICROSCOPY TECHNIQUES FOR BIOPHYSICAL QUESTIONS

In recent years tremendous progress has been made in the development of optical microscopy techniques. Many of these techniques represent promising approaches to address outstanding questions in biology and biophysical chemistry. The transition from a proof-of-principle technique to its actual implementation as a biological research tool, however, is challenging. This symposium aims to sketch a picture of the latest achievements in the application of advanced microscopy techniques to solve challenging biophysical and biological questions. In addition to highlighting the applications of advanced microscopy techniques, this symposium will also focus on emerging methods in microscopy with particular relevance to biological applications, including non-linear vibrational imaging, three-dimensional tracking, super-resolution imaging, and in vivo imaging.

Christine K. Payne, *Georgia Institute of Technology, christine.payne@chemistry.gatech.edu*
Eric O. Potma, *University of California, Irvine, epotma@uci.edu*

REDUCED DENSITY MATRICES IN QUANTUM CHEMISTRY AND PHYSICS

This symposium will employ reduced density matrices (RDMs) as a lens to view recent advances in quantum chemistry and physics. The following topics will be covered: (a) the description of strong electron correlation and entanglement in systems that are critical to our understanding of chemical and biological processes and reactivity as well as material science; (b) new methodologies in density functional theory and wavefunction methods and their connections to RDM methods; and (c) the use of RDMs in the study of molecular conductivity and light harvesting, non-Born-Oppenheimer nuclear motion, and quantum information and quantum molecular control. The symposium will provide a unique forum for participants to explore the important roles of RDMs throughout various areas of physical and theoretical chemistry.

David A. Mazziotti, *The University of Chicago, damazz@uchicago.edu*
Herschel A. Rabitz, *Princeton University, hrabitz@princeton.edu*
Neil Shenvi, *Duke University, neil.shenvi@duke.edu*

POSTDOCTORAL RESEARCH AWARDS

The PHYS Division plans to highlight leading research by postdoctoral fellows at the Fall National ACS meeting in Denver 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 24, so he/she can present at the meeting even if not selected for the special symposium. The deadline for applications is March 10, 2011, and selections will be announced shortly after the Spring ACS meeting in March 2011. More details on the award and applications procedure may be found at http://phys-acs.org.

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 Denver meeting. Up to 25 outstanding undergraduate chemistry students will be selected for a series of undergraduate-focused talks and social events during the Denver 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/UGworkshop11.html. The application deadline is February 11, 2011.

George Shields, *Bucknell University, george.shields@bucknell.edu*

On-Line Abstract Submission Deadline:
March 21, 2011
http://abstracts.acs.org

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

At the meeting in Denver, 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. 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.

SHARON HAMMES-SCHIFFER