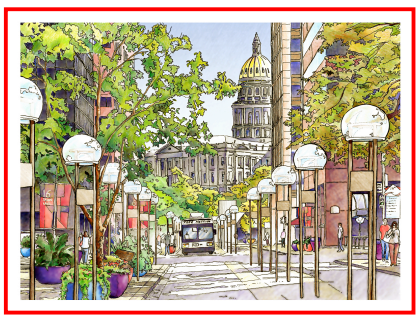
# ACS DIVISION OF PHYSICAL CHEMISTRY
## 249th NATIONAL MEETING, 22-26 March 2015
## DENVER, COLORADO
*THEME: Chemistry of Natural Resources*



# 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 August 25. **The abstract deadline is 20 October 2014**. 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.

### ROLE OF MEMBRANE IN AMYLOID-FORMATION AND THE PATHOGENICITY OF AMYLOID DISEASE

For decades, a central role for membranes has been proposed in the mechanism of amyloid formation and the pathogenicity of a number of amyloid diseases, including Alzheimer's Disease, Parkinson's Disease, and Type II Diabetes. Membranes have been proposed to play an essential role in (1) functional aspects of the processing of amyloid proteins, (2) catalyzing the early stages of amyloid protein aggregation, (3) facilitating intercellular amyloid propagation, and (4) the pathogenicity of amyloid disease involving channel/pore formation. In recent years, significant advances in experimental and computational approaches have made possible detailed studies of interactions of amyloid-forming proteins and lipid membranes. It is now increasingly possible to evaluate conjectures regarding the role of membranes in amyloid protein function and pathogenesis. This symposium will bring together research scientists from experimental biophysics (spectroscopy, NMR, microscopy) and computational biology (large-scale simulations, coarse-grained modeling, theory) to explore open questions in the field and identify the most promising approaches for future studies.

**Jennifer C. Lee**, *National Institutes of Health, leej4@mail.nih.gov*
**John E. Straub**, Boston University, straub@bu.edu

### DESIGN OF MATERIALS AND CHEMICAL PROCESSES: THE GENOMIC APPROACH

This symposium will explore recent development in the genomic approach to materials design and materials applications. We will discuss powerful paradigms for computationally-driven design and/or high-throughput-discovery of materials, including metallorganic frameworks and zeolites, that can be employed as superior new catalysts, for separation processes of central importance to our nation's energy future and energy security, and for gas storage. This symposium will bring together experts in quantum chemistry, classical simulation techniques and data mining and also a large number of experimentalists (ca 30% of the speakers are experimentalists) working in the area of catalysis and materials design and characterization.

**Laura Gagliardi,** *University of Minnesota gagliard@umn.edu*
**Berend Smit,** *University of California at Berkeley, berend-smit@berkeley.edu*

### CARBON IN THE GALAXY: THE FORMATION OF COMPLEX ORGANICS FROM THE OUTFLOW OF CARBON STARS AND THEIR EVOLUTION

Exploring the formation of complex organic molecules from the outflows of carbon stars and their evolution in various astrophysical environments is the theme of this symposium. Studying, through all interstellar stages, the formation, growth and destruction mechanisms of carbon containing species from simple molecules to cosmic dust grains is essential for a correct understanding of the role astrochemistry plays in planet formation and the primordial chemistry on that planet. Small carbon containing species dominate the astrochemical inventory of the gas phase compounds in dense molecular clouds, the cradles for star and planet formation. Larger, nanoparticle sized, complex organics influence many processes in the evolution of the interstellar medium itself such as the energy balance through the photoelectric effect, the ionization balance through recombination with electrons and reaction with molecular ions, and hence the chemical composition of molecular clouds.

**Louis J. Allamandola**, *NASA Ames Res. Center,* Louis.J.Allamandola@nasa.gov
**Timothy J. Lee**, *NASA Ames Research Center, Timothy.J.Lee@NASA.gov*

### ATMOSPHERIC CHEMISTRY SYMPOSIUM: TRANSFORMATIONS OF MATTER IN THE TROPOSPHERE

Chemical compounds emitted into the atmosphere readily undergo chemical and physical processing to form different gas and particulate phase compounds. The particulate phase species that result from atmospheric aging impact human health and influence climate through their interactions with radiation and clouds. This session focuses on all aspects of the transformations matter undergoes in the troposphere, including gas phase chemistry, aerosol nucleation, chemistry and phase separation in organic aerosol, aqueous chemistry, ice chemistry and nucleation, and heterogeneous chemistry. We will also emphasize experimental and theoretical efforts to understand the physical chemistry of these systems.

**Miriam Freedman**, *Penn State, maf43@psu.edu*
**Daniel Cziczo**, *MIT, djcziczo@mit.edu*

### MODELING EXCITED STATES OF COMPLEX SYSTEMS

Electronic excited states are crucial to the function of molecules and materials involved in fields with unavoidable complexity like solar energy conversion and biology. The accurate modeling of the behavior of even simple systems is challenging, because excited state potentials can be complex and unintuitive, and electronically excited systems are far from equilibrium, meaning dynamics can play a dominant role. This symposium focuses on large systems, complex environments, systems containing heavy elements, and states with multiply excited character. How can we model the dynamics of excited systems in a complex biological environment, the interacting potential energy surfaces of delocalized and localized excitations in extended materials, or the dynamics of spin-forbidden non-radiative processes? How do we accurately incorporate the interaction between states of singly and multiply excited character? This symposium will bring together experts with disparate methodological (electronic structure, molecular dynamics) and application (energy conversion, biology, catalysis, small molecule) expertise to stimulate discussion on these timely problems.

**Benjamin G. Levine**, *Michigan State University; levine@chemistry.msu.edu*
**Sergey A. Varganov**, *University of Nevada, Reno; svarganov@unr.edu*

### PROBING NANO-PLASMONIC PHENOMENA AT THE SINGLE MOLECULE, SINGLE ELECTRON, AND SINGLE PHOTON LEVEL

Harnessing the latest advances in electron and photon spectroscopy, microscopy, and scanning-probe techniques, nanoscale plasmonic phenomena are now routinely being interrogated below the difraction limit of light and manipulated toward desired responses with unprecedented spatial and spectral control. The distribution of energy between single nanoparticle aggregates and the single molecules that they support and their radiative farfield and thermal nearfield can be infuenced by the selective excitation of bright and dark plasmon modes, and their coupling into Fano resonances. Elucidating the basic physics that governs the plasmon's radiative and non-radiative decay pathways, particularly its decay into one or multiple hot electrons capable of initiating chemical transformations in the surrounding molecular environment, poses one of the next major challenges to the field, bearing significant impact upon chemical catalysis, nonlinear spectroscopy, and sensing. It is the purpose of this symposium to bring together both junior and senior experimentalists and theoreticians leading this effort to overview the latest advances in the field and to foster new ideas to direct and control nanoscale plasmonic phenomena at the single molecule, single electron, and single photon level.

**Stephan Link**, *Rice University, slink@rice.edu*
**David J. Masiello**, *University of Washington, masiello@uw.edu*
**Katherine A. Willets**, *University of Texas at Austin, kwillets@cm.utexas.edu*

### COMPUTATIONAL CHEMICAL DYNAMICS: ADVANCING OUR UNDERSTANDING OF CHEMICAL PROCESSES IN GAS-PHASE, BIOMOLECULAR, AND CONDENSED-PHASE SYSTEMS: A SYMPOSIUM IN HONOR OF DONALD TRUHLAR

This symposium will highlight the central role of theory and computation in our understanding of the structure, energetics, and dynamics of molecules in gas phase, macromolecular, and condensed-phase systems. It will emphasize theoretical and experimental studies that have advanced novel computational techniques and experiments validating theoretical results. In addition, this symposium will recognize contributions made by Professor Donald G. Truhlar and his collaborators in advancing computational tools and their application in these areas. Session are planned in the following areas: accurate energies for dynamics, gas-phase kinetics and dynamics, properties and processes in solvated systems, catalysis, nonadiabatic dynamics, enzyme kinetics and dynamics, and macromolecular dynamics.

**Bruce C. Garrett**, *Pacific Northwest National Laboratory, bruce.garrett@pnnl.gov*
**Jiali Gao**, *University of Minnesota, jiali@jialigao.org*
**Benedetta Mennucci**, *University of Pisa, benedetta.mennucci@unipi.it*

### MODELING COMPLEX BIOMOLECULES: FROM STRUCTURE TO DYNAMICS AND FUNCTION

Last year's Nobel Prize in Chemistry is at least in part a recognition for the increasingly central role played by molecular simulations in elucidating the connection between structure and function of biomolecules through studies of their dynamics. Molecular dynamics simulations have become indispensable tools in virtually all areas of biomolecular research, from the refinement of experimental structures to the interpretation of complex spectroscopic measurements, from the detailed analysis of atomic motions in enzymatic reactions to studies of the large-scale conformational dynamics in molecular machines and macromolecular folding. This symposium on "Modeling complex biomolecules: from structure to dynamics and function" aims to showcase these many roles of molecular simulations, by highlighting advances in key areas such as: the analysis and interpretation of complex biomolecular experiments, the studies of enzymatic reactions, the use of molecular simulations in quantitative studies of ligand binding and drug development, the function of molecular machines, and protein and nucleic acid folding.

**Angel E. Garcia**, RPI, angel@rpi.edu
**Gerhard Hummer**, Max-Planck Inst. of Biophysics, gerhard.hummer@biophys.mpg.de

### PHYSICAL ELECTROCHEMISTRY OF ELECTROCATALYTIC PROCESSES

Rapidly rising demands in energy and natural resources consumption combined with environmental pressures necessitate the move towards alternative sustainable sources and efficient use of our existing resources. Energy conversion technologies can help reduce dependence on non-renewable fossil fuels, lower greenhouse gas emissions, and enable more sustainable materials and resource choices. Nevertheless, current conversion technologies face several challenges such as energy efficiency, chemical selectivity, stability, and environmental impact. This symposium will explore the interfacial processes prevailing electrocatalytic reactions of small molecules such as $O_2$, $CO_2$, $H_2O$, alcohols and other small organic molecules at the electrode/electrolyte interface, relevant to advance electrocatalytic conversion technologies, such as fuel cells, electrolyzers with a specific focus on the following areas: (1) surface reactions (2) in situ characterization (3) theory and modeling.

**Anne Co**, *Ohio State University, co@chemistry.ohio-state.edu*
**Daniel Scherson**, *Case Western Reserve University, dxs16@case.edu*

### PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday evening, 25 March 2015. See announcement below for information about the Physical Chemistry Student Poster Awards.

**Ned Sibert**, *University of Wisconsin, sibert@chem.wisc.edu*

***On-Line Abstract Submission Deadline: 20 October 2014*** **http://abstracts.acs.org**

### PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

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.

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