



ACS DIVISION OF PHYSICAL CHEMISTRY
247th NATIONAL MEETING
DALLAS, TEXAS
THEME: *Chemistry and Materials for Energy*
16-20 March 2014



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 12. **The abstract deadline is 7 October 2013.** 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.

INTERFACES IN ENERGY STORAGE SYSTEMS

Interfaces at charged surfaces play a critical role for controlling the power and durability of electrochemical devices such as batteries and supercapacitors. Advanced *in situ* diagnostics are now focusing on interfacial layers with characteristic length scales of tens of nm (solid-electrolyte interfaces, SEI) or tens of Angstroms (electric double layer). Simultaneously, advanced theoretical developments provide interpretations of these experiments as well as new predictions of the chemical, transport, and mechanical processes that occur at electrified interfaces. These approaches will, for the first time, elucidate the microscopic mechanisms dictating cell life and performance. The goal of this symposium is to foster these new efforts to understand these physical-chemical processes.

Stephen Harris, Lawrence Berkeley National Lab, harris.stevharris@gmail.com
David Limmer, University of California, Berkeley, dlimmer@berkeley.edu
Kristin Persson, Lawrence Berkeley National Laboratory, KAPersson@lbl.gov

**A LITTLE INSIGHT GOES A LONG WAY: A TRANSFORMATIVE
ROLE OF THEORY IN SPECTROSCOPY AND CHEMICAL
DYNAMICS**

"The purpose of computing is insight, not numbers" ... R.W. Hamming

The symposium will highlight a transformative role that theory plays in modern research by making bold predictions, guiding the design of new experiments, and enabling insightful interpretation of experimental observations. The focus of the symposium will be on the theories and computational approaches connecting experimental observations to the underlying interactions between atoms and molecules developed by Prof. Benny Gerber and his colleagues, collaborators, students, and post docs. The topics will cover a broad range of experimental and theoretical physical chemistry including atmospheric processes, novel rare gas containing compound, new spectroscopic approaches, and more.

Anna I. Krylov, University of Southern California, krylov@usc.edu
Masha Y. Niv, The Hebrew University of Jerusalem, niv@agri.huji.ac.il
Susan K. Gregurick, Dept. of Energy, susan.gregurick@science.doe.gov
Anne B. McCoy, Ohio State University, mccoy@chemistry.ohio-state.edu

**ULTRAFAST PROCESSES IN PROTEINS:
THEORY AND EXPERIMENT**

Incomplete understanding of light-triggered processes in proteins imposes severe limits in harnessing biological activity to generate useful functions such as solar energy conversion, vision, photo-transduction, gene-regulation and gene-repair. Similar understanding is required for the engineering of novel photoactive materials including genetically encoded optical probes and light-responsive receptors/actuators. The primary photodynamics extending from femtoseconds to picoseconds is central to the efficiency of these processes and requires the use of advanced ultrafast spectroscopies and state-of-the-art quantum chemical computations to be adequately studied. This symposium will provide an overview of the current advancements in ultrafast protein dynamics, both theoretical and experimental, necessary to reconstruct the mechanisms underlying the photoactivated responses of proteins including photosystems, flavoproteins, rhodopsins, photoenzymes, fluorescent proteins, and their corresponding chromophores.

Delmar Larsen, University of California Davis, dlarsen@ucdavis.edu
Massimo Olivucci, Bowling Green State University/Sienna University, molivuc@bgsu.edu

**THERMODYNAMICS, REACTIVITY, AND SPECTROSCOPY OF
THE HEAVY ELEMENTS**

Compounds of heavy elements, lanthanides and actinides, have unique magnetic, catalytic, and luminescent properties. They are critical to energy technologies, including solar panels, solar hydrogen production, wind turbines, electric vehicles, energy-efficient lighting, and nuclear technologies. Furthermore, they have important catalytic properties. In order to be able to design materials that are efficient and safe to use, it is essential to have greater insight about the thermodynamics, reactivity, and spectroscopy of heavy element materials and compounds. This symposium will focus upon both theoretical and experimental efforts and developments towards better understanding these properties.

Angela K. Wilson, University of North Texas, akwilson@unt.edu
Paul Bagus, University of North Texas, bagus@unt.edu
Laura Gagliardi, University of Minnesota, gagliard@umn.edu
Hicham Idriss, Saudi Basic Industries Corporation, CRI/KAUST, idriss@h@h@sabic.com

**PHYSICAL CHEMISTRY OF LOW DIMENSIONAL
NANOMATERIALS: FROM DOTS TO WIRES TO SHEETS**

This symposium will focus on experimental and theoretical advances in the size-, shape- and dimensionality-dependent optical and electrical properties of nanoscale materials. Our focus will include quantum dots, nanoclusters, nanowires and layered materials. Also of interest are hybrid systems based on mixed compositions or mixed dimensionalities made through bottom-up chemistries. Submissions on ensemble as well as single nanostructure imaging and spectroscopic techniques with high spatial and/or temporal resolution are encouraged. Given the rapid growth of nanostructure applications, fundamental studies covering the fate of photogenerated charges and other excitations will represent another major topical thrust of the symposium.

Masaru Kuno, Notre Dame University, Masaru.K.Kuno.1@nd.edu
Rongchao Jin, Carnegie Mellon University, rongchao@andrew.cmu.edu
Matthew Sfeir, Brookhaven National Laboratory, msfeir@bnl.gov

IN SITU STUDIES OF FUEL CELL MATERIALS AND DEVICES

The need for clean and efficient production of electrical power has motivated rapid progress in fuel cell (FC) development. However, formidable hurdles must still be overcome before FCs are ready for widespread commercial development. This symposium will highlight recently developed methods that characterize and quantify elementary oxygen reduction and fuel oxidation reactions as well as contaminant poisoning and mechanisms responsible for device failure with an emphasis on solid oxide fuel cells (SOFCs) and proton exchange membrane fuel cells (PEMFCs). The interplay between *in situ* experimental findings and the development of detailed kinetic models designed to optimize device performance and minimize material degradation will be a common theme throughout the symposium.

Robert A. Walker, Montana State University, rawalker@chemistry.montana.edu
Jeffrey C. Owrutsky, Naval Research Laboratory, jeff.owrutsky@nrl.navy.mil

CLUSTERS IN CATALYSIS

Small clusters of transition metals are intriguing species with unexpected electronic structures. Those are manifested in specific and highly tunable properties of clusters, such as catalytic activity that depends strongly and non-linearly on cluster size and composition. The symposium will focus on small clusters, both stand-alone, and as parts of catalytic materials, understanding the relationships between the electronic structure of these clusters and their catalytic activities, and further rational manipulation of the latter through the former. We hope to facilitate the discussion between people from the entire spectrum of cluster science, from fundamentals to industrial applications.

Anastassia N. Alexandrova, University of California, Los Angeles, ana@chem.ucla.edu
Mark Saeys, National University of Singapore, saeys@nus.edu.sg

**CHEMISTRY IN THE INTERSTELLAR MEDIUM:
NEW FRONTIERS IN LABORATORY, THEORY, AND
OBSERVATIONS**

This symposium highlights interdisciplinary astrochemistry research efforts with the ultimate goal of elucidating the chemistry of the interstellar medium. Topics for this symposium include results from recent molecular observations, laboratory investigations of chemical reaction dynamics in gases, ices, and on surfaces, laboratory spectral studies of interstellar molecules, kinetic modeling of the chemistry of interstellar clouds, and laboratory and observational studies of large molecules. These topics cover state-of-the-art spectroscopy, kinetics, and dynamics experiments, complemented by theoretical predictions, allowing a characterization of the elementary reactions that also occur during the processes of star- and planet-formation.

Eric Herbst, University of Virginia, eh2ef@virginia.edu
Ralf I. Kaiser, University of Hawaii, ralfk@hawaii.edu
Susanna Widicus Weaver, Emory University, susanna.widicus.weaver@emory.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, 19 March 2014. See announcement below for information about the Physical Chemistry Student Poster Awards.

Nancy Levinger, Colorado State University, Levinger@lamar.colostate.edu

On-Line Abstract Submission Deadline: 7 October 2013
<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.

NANCY LEVINGER, PROGRAM CHAIR
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