



ACS DIVISION OF PHYSICAL CHEMISTRY 252ND NATIONAL ACS MEETING

Philadelphia, PA 21-25 August 2016

Meeting Theme: "Chemistry of the People, By the People, and For the People"



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. **The abstract deadline is 21 March 2016.** 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.

PHYSICAL CHEMISTRY MEETS AMO

There is a long history of experimental and theoretical techniques being transferred between physical chemistry and atomic physics. Recently modern atomic physics techniques such as laser-cooling, Bose-Einstein condensation, and cold ion crystals have been applied to molecular systems. Progress in the last few years has been impressive with demonstrations of isomer dependent chemical reactions, condensates of neutral molecules, and molecular ions in their ground state of motion. The goal of this symposium is to bring together researchers from both the physics and chemistry communities to discuss recent advances and to seed future collaborations.

Kenneth Brown, *Georgia Tech*, ken.brown@chemistry.gatech.edu

Michael Heaven, *Emory University*, heaven@euch4e.chem.emory.edu

PHYSICAL CHEMISTRY OF ATMOSPHERIC PROCESSES

Results from laboratory, ambient, and theoretical investigations of atmospherically important chemical processes continue to challenge our understanding of physical chemistry. Our knowledge of the kinetics and mechanisms of gas-phase radical reactions, reactions at interfaces, multiphase chemical reactions, nucleation and growth of aerosols, and the atmospheric processing of natural and anthropogenic emissions is constantly improving due to exciting advances in laboratory, field, and theoretical techniques. However, numerous questions still remain regarding the impacts of chemistry on air quality and climate via mechanisms such as ozone formation, oxidation of organic and inorganic species, aerosol nucleation and growth, and aerosol optical, hygroscopic, and cloud nucleating properties. This symposium will bring together researchers from these aforementioned areas to discuss recent advances and to identify future research directions.

Paul Ziemann, *University of Colorado Boulder*, paul.ziemann@colorado.edu

Ellie Browne, *University of Colorado Boulder*, eleanor.browne@colorado.edu

FRONTIERS OF SOLAR SYSTEM CHEMISTRY: PLANETS TO COMETS AND BEYOND

This symposium will focus on the chemistry associated with the origin, evolution, and present state of the Solar System. Surface, sub-surface, and atmospheric chemistry will be highlighted through contributions by laboratory scientists, theorists, and astronomical observers. Presentations will cover the chemistry of planets as well as that of small bodies, such as planetary satellites, comets, asteroids, meteors, and trans-Neptunian objects. Contributions from research teams investigating the chemistry of Mars with the Mars Science Laboratory's Curiosity rover, of comets with the European Space Agency's Rosetta mission, of asteroids with NASA's OSIRIS-REx mission, and of the outer Solar System with the New Horizons spacecraft are planned. Exciting ALMA radio-telescopic observational results for Titan and other objects are encouraged for this session, along with glimpses at what chemical discoveries await with the James Webb Space Telescope. The symposium also aims to promote discussion of laboratory and theoretical needs of the astronomy and planetary-science communities.

Reggie Hudson, *NASA Goddard Space Flight Center*, reggie.hudson@nasa.gov

Stefanie N. Milam, *NASA Goddard Space Flight Center*, stefanie.n.milam@nasa.gov

ADVANCED POTENTIAL ENERGY SURFACES

Advanced potential energy surfaces, defined as classical or quantum mechanical treatments beyond widely available classical fixed charge pairwise-additive force fields, are encountering obstacles that inhibit their application to grand challenge chemistry problems: limitations of accuracy, computational cost of the theoretical models, lack of innovation in approximate polarizable models and algorithms that can mitigate the cost, limited dissemination to a broad range of community codes, under-developed software interfaces between theoretical models, and lagging quality software implementations on HPC architectures and newer GPU and multicore hardware. We propose to invite a broad cross section of the theoretical and computational chemistry community that are working on overcoming these obstacles and involved in chemical and biochemical applications, advanced force field development, electronic structure methods applied to QM/MM, molecular dynamics algorithms, and software development.

Teresa Head-Gordon, *University of California, Berkeley*, thg@berkeley.edu

Chris Skylaris, *University of Southampton*, c.skylaris@soton.ac.uk

ACCELERATING DISCOVERY: CITIZEN SCIENCE, BIG DATA, AND MACHINE LEARNING FOR PHYSICAL CHEMISTRY

The nature of computational chemistry is undergoing an unexpected transformation: The available computing time is growing dramatically and presents itself in new ways (including cloud and grid resources). Unprecedented quantities of data are being generated in high-throughput screening projects and made available to the community through open databases. Machine learning and other techniques from modern data science are finding their way into chemistry to extract insights from these data sets, and the focus thus shifts from the study of individual molecules to the exploration of chemical space. Many challenges and opportunities are arising in this context. This symposium will showcase innovative approaches from many areas of chemistry and materials science that are on the forefront of all these new developments.

Alán Aspuru-Guzik, *Harvard University*, alan@aspuru.com

Johannes Hachmann, *SUNY, University at Buffalo*, hachmann@buffalo.edu

IMPACTS OF NANOTECHNOLOGY AND SINGLE MOLECULE SPECTROSCOPY IN BIOLOGY AND MEDICINES

This interdisciplinary symposium will highlight recent advances in nanotechnology and single molecule spectroscopy, and their unique applications in biology and medicine. Advances in nanotechnology have enabled us to study the interface of biological system and nanomaterials, to develop new imaging probes for better understanding of cellular functions, and to design novel medicines and biomaterials for more effective disease diagnosis and therapy. Single molecule spectroscopy enables us to explore cellular living organisms at individual molecule resolution and with single molecule sensitivity, to characterize structures and functions of single macromolecules (protein) at nanoscale, to depict rare biological events and phenomena, to offer new insights into cellular functions, and to provide molecular tools for sensing and detecting of rare subsets of single cancer cells in highly heterogeneous cellular population. This symposium will gather pioneers and rising stars now leading the development and applications of these emerging enabling technologies and showcase the latest development of this new frontier.

X. Nancy Xu, *Old Dominion University*, xhxu@odu.edu

METAL AND SEMICONDUCTOR NANOCCLUSERS WITH ATOMIC PRECISION: FUNDAMENTALS AND APPLICATIONS

This symposium will focus on the research advances in metal and semiconductor nanoclusters, ranging from the synthesis to studies of fundamental properties and applications. Atomically precise nanoclusters have provided many opportunities for discovering new properties and developing exciting applications and are expected to serve as paradigm systems to shed light on the unsolved issues in metal/semiconductor nanoparticles such as nucleation, size evolution and precise surface chemistry. This symposium will bring together experimentalists and theoreticians in hope of fostering collaborations between researchers from various disciplines. The multi-day sessions will blend the synthesis people in new materials making, experimentalists specialized in physicochemical measurements and function studies, and theoreticians providing insights in the electronic structures for structure-function correlations.

Rongchao Jin, *Carnegie Mellon University*, rongchao@andrew.cmu.edu

Gangli Wang, *Georgia State University*, glwang@gsu.edu

Jie Zheng, *The University of Texas at Dallas*, jiezheng@utdallas.edu

Matthew Sfeir, *Brookhaven National Lab*, msfeir@bnl.gov

ADVANCES IN BIOLOGICAL IMAGING

In recent years, significant advances in the methodologies of biological imaging have enabled us to resolve biological features and structures with unprecedented spatial resolution and chemical specificity. Methodologies that were developed for simple and well-behaved inorganic substrates and materials are increasingly being applied to complicated biological samples in physiologically relevant environments and matrices thanks to innovations in both instrumentation and sample preparation methods. Through these innovations, entirely new insights have become possible, leading to molecular-level resolution of complex and heterogeneous biological materials and systems. This symposium will focus on bioimaging achievements based on techniques including scanning probe and super-resolution microscopies and mass spectrometry. The goal of this symposium is not just to highlight methodological advances—but to promote discovery and discussion of the relevant biological insights that have been gained from the spatial and chemical resolution these technologies afford.

Lauren Webb, *University of Texas*, lwebb@cm.utexas.edu

Julie S. Biteen, *University of Michigan*, jsbiteen@umich.edu

Amanda Hummon, *University of Notre Dame*, ahummon@nd.edu

DYNAMICS OF NATURAL AND ARTIFICIAL SYSTEMS FOR ENERGY CONVERSION: INSIGHTS GAINED FROM SPECTROSCOPIC METHODS AND THEORY

This symposium will serve to outline recent advances in our understanding of the dynamics of (1) natural and artificial photosynthetic systems and (2) photovoltaic materials and devices. The symposium aims to bring together researchers whose expertise spans the fields of ultrafast spectroscopy, microscopy, and theoretical approaches in order to discuss a wide range of topics relevant to harvesting and controlling energy flow, including biophysical processes, structural dynamics, energy transfer, electron transfer reactions, and yield of energy conversion processes. The main objectives of the symposium will be to discuss recent advances pertaining to our understanding of the dynamics of natural biological and biomimetic systems and photovoltaic materials and devices, along with outlining the next experimental and theoretical challenges that are relevant to harvesting and controlling energy flow.

Jessica M. Anna, *University of Pennsylvania*, jmanna@sas.upenn.edu

Michael R. Wasielewski, *Northwestern University*, m-wasielewski@northwestern.edu

Abraham Nitzan, *University of Pennsylvania*, anitzan@sas.upenn.edu

INTRINSICALLY DISORDERED PROTEINS: STRUCTURE, FUNCTION, AND INTERACTIONS

This symposium will highlight recent work elucidating the link between the biophysical properties of disordered proteins and their structure and function, as well as the methodological advances enabling these breakthroughs. Emphasized topics include (i) state-of-the-art predictive computational models validated by experimental observables which can provide molecular details of disordered structural ensembles as well as kinetic information on structural rearrangements, (ii) application of both single-molecule and atomic resolution techniques to obtain quantitative information on structural and dynamical properties, and (iii) disordered protein interactions including physiological liquid-liquid phase separation. A primary goal will be to bring together researchers working in theory, simulation, and experiment. This synthesis will lead to advances in understanding of how the physical properties of disordered proteins direct physiological function, disease-associated dysfunction, and can be engineered in new materials or targeted for novel therapeutics.

Jeetain Mittal, *Lehigh University*, jeetain@lehigh.edu

Nicolas Fawzi, *Brown University*, nicolas_fawzi@brown.edu

PHYS DIVISION RESEARCH AWARDS AND JPC LECTURESHIP AWARDS

The four winners of the PHYS Division Research Awards and the three winners of the Journal of Physical Chemistry Lectureship Awards will present talks at this one-day symposium.

PHYSICAL CHEMISTRY SYMPOSIUM WORKSHOP FOR UNDERGRADUATE CHEM MAJORS

The Workshop for Undergraduate Chemistry Majors is targeted for current junior chemistry majors who will be seniors at the time of the Philadelphia meeting. Up to 25 outstanding undergraduate chemistry students will be selected for a series of undergraduate-focused talks and social events during the Philadelphia 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://phys-acs.org/ugrad_workshop/2016.html. The application deadline is **26 February 2016**.

Casey Londergan, *Haverford College*, clonderg@haverford.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, 24 August 2016. See announcement below for information about the Physical Chemistry Student Poster Awards.

Greg Engel, *University of Chicago*, gsengel@uchicago.edu

On-Line Abstract Submission Deadline: 21 March 2016

<http://abstracts.acs.org>

POSTDOCTORAL RESEARCH AWARDS

PHYS Division Postdoctoral Research Awards and invited talks will be presented at the relevant PHYS Symposia.

PHYSICAL CHEMISTRY STUDENT POSTER AWARDS

Six 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 and must be present during judging.

GREGORY S. ENGEL, PROGRAM CHAIR **University of Chicago** (773) 834-0818 gsengel@uchicago.edu

FOR INFORMATION ABOUT THE PHYSICAL CHEMISTRY DIVISION. VISIT OUR WEBSITE: <http://phys-acs.org/>