ACS DIVISION OF PHYSICAL CHEMISTRY
250TH NATIONAL MEETING
Boston, Massachusetts
16-20 August 2015

Meeting Theme: Innovation From Discovery To Application

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 27 March 2015**. 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.

ELECTRONIC STRUCTURE THEORY FOR LARGE SYSTEMS

The gradual increase in computing power alone (Moore's law) will be insufficient, in our lifetimes, to defeat the highly non-linear scaling of ab initio quantum chemistry. To extend such methods to hundreds or thousands of atoms, innovative algorithms and novel implementations of existing ones are required. This is true both at the level of the quantum mechanics itself (seeking more efficient approximations to the electron correlation problem) but also at the level of scalable-parallel implementations of new and existing algorithms. This symposium will bring together developers focused on extending quantum chemistry for application to larger systems. Topics will include (1) scalable-parallel implementations of quantum-chemical methods; (2) fragment-based approaches that are embarrassingly parallelizable for distributed computing; (3) linear-scaling algorithms and local correlation techniques; and (4) condensed-phase ab initio molecular dynamics simulations.

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MATERIALS FOR HEAT TO ENERGY CONVERSION

The symposium will highlight cutting-edge research in the discovery and applications of innovative materials that lead to high conversion efficiency for heat-to-energy conversion. The symposium is designed to emphasize the multidisciplinary nature (chemistry, materials science, physics, engineering) of the research needed to advance the state-of-the-art technologies for energy conversion. A main focus will be on recent material and technological innovations in the fields of thermoelectrics, thermionics, and solar-thermal routes. Chemical, thermal, electrical, and device properties of materials will be emphasized. Theoretical studies of transport properties, band structure, and crystal chemistry of materials, thermodynamic analysis, and energy transfer in various processes will also be emphasized.

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CHEMICAL PROCESSES OF ATMOSPHERICALLY RELEVANT TRACE GASES, AEROSOLS AND CLOUDS

The atmosphere represents an environment full of complex chemical interactions between gaseous species, aerosol particles and clouds. Aerosol particles derived from primary anthropogenic or biogenic sources or stemming from secondary processes are ubiquitous in the atmosphere. Recently there have been major advances in our understanding of such multiphase processes involving aerosols and clouds. However, more knowledge is needed for a comprehensive understanding of the aerosol-cloud life cycle such as quantification of the trace gases involved and the morphology and phase state of aerosol particles with subsequent consequences for water uptake, reactivity and optical particle properties, and cloud processing of aerosol. The session will gather researchers from the field and laboratory, aerosol scientists and atmospheric modelers with the goal of disentangling the intertwined chemical processes and identifying needed research in atmospheric chemistry.

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FROM DIRADICALS AND POLYRADICALS TO FUNCTIONALIZED MATERIALS: THEORY MEETS EXPERIMENT

Diradicals and polyradicals play an increasingly important role in unconventional chemical reactions and for the design of advanced materials. Highly topical and fascinating research fields range from engineering graphene nanoflakes to organic superconductors, high-spin polyradicals, molecular magnets, photo-induced switches, chemical sensors and bio-organic reactions with promising applications in the material sciences. The accurate characterization of the chemical reactivity and the control of the molecular properties of these systems are crucial for the improvement of current technologies and for the development of new lead applications. The symposium aims at providing an overview of the state-of-the-art both in theoretical and experimental investigations in the mentioned fields and offering a discussion forum to advance the multidisciplinary research and to foster new ideas.

Hans Lischka, *Texas Tech University*, Hans.Lischka@ttu.edu
Carol Parish, *University of Richmond*, cparish@richmond.edu
Miklos Kertesz, *Georgetown University*, kertesz@georgetown.edu

HYDROPHOBICITY, ION SOLVATION, AND INTERFACES: THEORY, SIMULATIONS, AND EXPERIMENTS

Water is, perhaps, the most important material in the world – fascinating even in its pure state for the range of anomalous properties it displays. There has been an increasing realization that understanding the behavior of water near solutes, ranging from small hydrophobic and ionic solutes to biomolecules and interfaces holds the key to understanding water-mediated interactions, recognition, and self-assembly. Impressive advances have been made over the past few years using theory, simulations, and experiments toward understanding of hydrophobicity, ion hydration and interactions, as well as interactions and assembly at interfaces. These advances are at the core of the physical chemistry of aqueous solutions and lie at the interface of chemistry, biology, chemical engineering, and materials science.

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MOLECULAR BIOPHYSICS: REVEALING THE INTERPLAY BETWEEN DIFFERENT FORCES AND EFFECTS IN BIOCHEMICAL PROCESSES

Many biochemical processes are governed by the precise balance of various forces and effects, with electrostatics frequently paying significant role. These processes include protein, membrane, RNA and DNA folding, stability, and interactions, and associated proton and electron transport. They occur in water, which further complicates theoretical and experimental investigations. In some cases the water phase can be treated as a homogeneous a medium, while in others the individual water molecules must be considered. The goal of this symposium is to bring together computational and experimental researchers with common interests in Molecular Biophysics, particularly those whose investigations focus on revealing the role of the water phase in biological reactions. A symposium with researchers utilizing and developing different experimental and computational methods certainly helps reveal the strengths and weaknesses of these approaches and will lead to further improvements.

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STRUCTURE AND DYNAMICS IN COMPLEX CHEMICAL SYSTEMS: GAINING NEW INSIGHTS THROUGH RECENT ADVANCES IN TIME-RESOLVED SPECTROSCOPIES

The intricacy of most chemical, biochemical, and material processes and their applications are underscored by the complex nature of the environments in which they occur. Substantial challenges for building a global understanding of a heterogeneous system include (1) identifying unique signatures associated with specific structural motifs within the heterogeneous distribution, and (2) resolving the significance of each of multiple time scales involved in both small- and large-scale nuclear reorganization. This symposium focuses on the progress in our understanding of dynamics in complex systems driven by recent innovations in time-resolved spectroscopies and theoretical developments. Such advancement is critical for driving discovery at the molecular level facilitating new applications. Broad areas of interest include: Structural relaxation and the impact of structure on dynamics in liquids, interfaces, biochemical systems, materials, and other heterogeneous environments.

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THE PHYSICAL CHEMISTRY OF CLUSTERS AND NANOPARTICLES

This symposium will provide an overview of ongoing developments in the synthesis, controlled deposition, characterization, and application of size-selected clusters and nanoparticles. These materials exhibit structural, reactive, optical, and magnetic properties that may vary substantially with size, composition, surface coverage, and interaction with an underlying support. We will discuss cutting-edge experimental techniques for preparing and characterizing size-selected clusters and nanoparticles as well as state-of-the-art theoretical methods for calculating the geometric structure and electronic properties of these well-defined species. The objective is to explore structure-function relationships that may be applied to direct the design of cluster-based materials with tailored properties for a variety of applications including catalysis, energy storage, and nanoelectronics. We aim to promote discussion between researchers working in several areas pertaining to clusters and nanoparticles to achieve a holistic understanding of these novel materials.

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PROTEIN-NANOMATERIAL INTERFACES AND PROTEIN CORONAS: PHYSICAL PROPERTIES, BIOCOMPATIBILITY, AND BIOLOGICAL IMPACT

The synergistic combination of nanotechnology and biology has resulted in numerous innovative approaches for therapy and biology. One of the biggest issues for effective use of nanoparticles in biology is the interface between the nanomaterial and its biological environment. When nanoparticles are introduced to biological fluids, the proteins and other species present non-specifically adsorb to their surfaces, forming a "protein corona." The corona can block the surface of the nanoparticle, cause undesired side effects in targeting, biocompatibility, biodistribution, and other biological consequences. Probing the nanomaterial-protein interface poses unique challenges, as interactions are weak and constantly evolving. This symposium will focus on the interface of nanomaterials with biomolecules, cells, biological fluids, properties of protein coronas, protein- and DNA-nanoparticle interactions, as well as the impact of the nanomaterial-biological interface on biocompatibility, biodistribution, *in vitro* and *in vivo* toxicity.

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Clemens Burda, *Case Western Reserve University*, cxb77@case.edu
Wolfgang Parak *Univ. Marburg, Germany, and CIC Biomagune, Spain*, wolfgang.parak@physik.uni-marburg.de

BRINGING ASTROCHEMICALS BACK TO EARTH: FORMATION MECHANISMS, STABILITY, AND SPECTROSCOPIC SIGNATURES

Our knowledge of chemistry is largely limited to those reactions that take place under standard terrestrial surroundings with little variation beyond Earth's ambient conditions. However, this is but a fraction of all possible chemical environments. By exploring the innumerable physical settings observable in the universe, it is possible to examine how chemistry can take place in seemingly bizarre and alien environments. It is within these challenging environs that new science is pioneered. This science does not have to remain in space but can be applied to develop new chemical understanding here on Earth. This symposium focuses on how non-terrestrial conditions can play a role in the development of new molecules, pathways, and experiment design. It is open to the discussion of new experimental techniques, theoretical and computational developments, and novel chemicals pioneered with an aim for applications of these astrochemically-derived breakthroughs to other areas of chemistry.

M. Samy El-Shall, *Virginia Commonwealth University*, mselshal@vcu.edu
Ryan C. Fortenberry, *Georgia Southern University*, rfortenberry@georgiasouthern.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 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://phys-acs.org/ugrad_workshop/2015.html. The application deadline is February 10, 2015.

Carol Parish, University of Richmond, PHYSworkshop@richmond.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 August 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: 27 March 2015 **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.

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