CALL FOR PAPERS

ACS DIVISION OF PHYSICAL CHEMISTRY

258th NATIONAL ACS MEETING

San Diego, CA ☺ 25-29 August 2019

Meeting Theme: "Chemistry & Water"

The Division of Physical Chemistry has organized the following oral symposia, consisting of both invited and contributed papers, as well as topical and general poster sessions. **The abstract submission deadline is 18 March 2019**. 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.

WATER IN THE UNIVERSE

Formed from two of the most abundant elements in the universe, the special chemical and physical properties of water make it a uniquely important molecule in the quest to understand our origins. Dramatic advances in observational capabilities from millimeter-wave to infrared wavelengths and in our ability to study water vapor, liquid water, and water ice from first principles calculations and with ever more capable laboratory methods now enables astronomers, planetary scientists and chemists to follow the 'water trail' from the interstellar medium to mature (exo)planetary systems. With a strong focus on the chemistry of, and enabled by, water, and the interplay between studies of our own and exoplanetary systems, this symposium will highlight the cosmic history of water, its critical role in the formation and early evolution of planetary systems, and the means by which habitable environments are created across the Universe. Topics will include water at cosmic distances, water in the interstellar medium, in planetary disks and in the Solar System, and water in exoplanetary systems.

Geoffrey A. Blake, *California Institute of Technology*, gab@gps.caltech.edu
Sergio Ioppolo, *Queen Mary University of London*, s.ioppolo@gmul.ac.uk

GETTING TO THE BOTTOM: OPTICAL AND ELECTRON IMAGING OF REACTIVE CHEMICAL SYSTEMS

Much of our current understanding of complex reactive chemical systems, whether a living organism or a working battery, comes from experimental measurements of macroscopic behavior. It is generally unclear how individual components in a complex chemical network communicate at the atomic and molecular levels, and how these interactions ultimately lead to system function. This symposium will bring together chemists who are interested in "getting to the bottom" of the chemistry underlying real-world applications ranging from human health to energy production and storage using the methods of experimental physical chemistry. This symposium will encompass the latest developments in temporally and spatially resolved optical and electron spectroscopy techniques applied to a wide range of molecules, interfaces, and materials. Speakers include experts in areas ranging from energy generation and storage to cell biology.

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HYDRATION FROM THE GAS TO THE CONDENSED PHASE

This symposium will focus on experimental and theoretical progress in our understanding of hydration structure and dynamics from small clusters in the gas phase to aqueous solutions and interfaces. We will discuss recent developments and applications of experimental techniques, theoretical models, and simulation approaches to the molecular-level characterization of structural, thermodynamic, and dynamical properties of aqueous systems across different phases, in different environments, and under different temperature/pressure conditions. Specific focus will be on the relationship between spectroscopic signatures and underlying structure/dynamics of the hydrogen bond network. We will highlight recent experimental work obtained with static, phase- and time-resolved spectroscopic methods, as well as advances in the representation of molecular interactions, data-driven algorithms, and simulation techniques that have recently enabled the study of complex solutions with an unprecedented level of accuracy and detail. This session provides a unique platform for discussing various aspects of the hydration structure and dynamics in the gas-phase, liquid-phase, and interface. By updating the progress in each of these fields, we aim to share the knowledge between these fields, thereby contributing to networking within the larger community, and stimulating interdisciplinary collaborations.

Ellen Backus, *Max Planck Institute for Polymer Research,* backus@mpip-mainz.mpg.de
Mischa Bonn, *Max Planck Institute for Polymer Research,* bonn@mpip-mainz.mpg.de
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PHYSICAL CHEMISTRY OF THE ATMOSPHERE

Many of the atmospheric processes central to air quality, human health, and climate – including the formation of particulate matter, the degradation and transformation of pollutants, the absorption and scattering of light by gases and particles, and the formation of cloud droplets – are controlled by a complex interplay of chemical reactions, photolytic processes, and phase changes. A detailed understanding of these processes is critical for accurate modeling of atmospheric composition and prediction of climate and air quality. This symposium explores the properties and evolution of atmospheric constituents. Specific topics include nucleation (forming new particles, cloud droplets, and ice crystals), the properties of particulate matter (phase, viscosity, water uptake, and optical properties), the chemical processes controlling radical concentrations, and the chemical transformations of organic compounds in both the gas and condensed phases.

Akua Asa-Awuku, *University of Maryland,* asaawuku@umd.edu
Miriam Freedman, *Pennsylvania State University,* maf43@psu.edu
Jesse Kroll, *Massachusetts Institute of Technology*, jhkroll@mit.edu

RECENT DEVELOPMENTS IN BIOMATERIALS

The symposium will present recent development in the field of biomaterials with a focus on communicating latest developments in: 1) fundamental understanding in biomaterial behavior under relevant biological condition; 2) synthetic biology, soft material synthesis, characterization and potential implementation toward new classes of biomaterials; 3) ability to control self-assembly over multiple length scales and time scales to better interface with biological systems; 4) improved knowledge in kinetic pathway and non-equilibrium states in biomaterials. This symposium will gather people from different disciplines with a central theme of achieving basic understanding in and, ultimately, controlling how materials behavior under biological condition spatially and temporally. The interdisciplinary symposium will provide a venue for bringing to light the latest developments in fields such as living polymerization with certain monomer sequence control, synthetic biology with increasing knowledge at single cell level, various characterization techniques enabling probing bio/abiotic interface with unprecedented resolution and directed self-assembly capable of accessing nonequilibrium states.

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AT THE INTERFACES OF EXPERIMENTAL AND THEORETICAL NONLINEAR OPTICAL MOLECULAR SPECTRO-IMAGING

The rapid development of nonlinear optical molecular spectroscopy/microscopy has provided fundamental molecular insights into biological systems, energy materials and chemical sciences. A joint force from both experimental and theoretical approaches can push the boundary of science that neither approach can achieve by itself. This symposium will bring together experts in the field of nonlinear optical spectroscopy and microscopy with the goal of stimulating discussion and synergies of further integrating experimental and theoretical research to investigate complex molecular systems in various aspects. Topics of interest include: development & applications of coherent multidimensional spectroscopy for molecular spectra and dynamics, interface sensitive optical spectroscopy for complex molecular interfaces, integration of nonlinear spectroscopy with new light sources (HHG, FEL, frequency combs, THz sources etc.), hyperspectroscopic imaging for resolving spectra and dynamics of molecular systems.

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NANOSCALE AND MOLECULAR ASSEMBLIES: DESIGNING MATTER TO CONTROL ENERGY TRANSPORT

Recent experimental, theoretical and computational advances have enabled the design and realization of molecular and nanostructured assemblies with novel, complex, and often unusual electromagnetic properties unattainable in their individual constituents. Such assemblies provide unique opportunities to manipulate energy flow in a variety of regimes, from the electronic and excitonic energy flow initiated by UV and visible excitation to vibrational and phononic energy flow initiated by IR, terahertz, and microwave excitation. Contributions may highlight recent progress in the physical understanding, experimental realization, or application of molecular and nanostructured assemblies towards controlling energy flow at molecular and nanoscaled dimensions; talks that develop or utilize theoretical and/or computational methods towards these ends are also welcome.

Justin Caram, *University of California, Los Angeles*, jcaram@chem.ucla.edu
Jay Foley, *William Patterson University*, foleyj10@wpunj.edu
Dugan Hayes, *University of Rhode Island*, dugan@uri.edu

TOWARD CHEMISTRY IN REAL SPACE AND TIME

The symposium is organized by the NSF Center for Chemistry at the Space-Time Limit, in its sunset year. It will focus on science aimed at visualizing molecular dynamics and chemistry at the ultimate limits of resolution in space and time and with sensitivity reaching the single molecule limit. The symposium will principally focus on near-field techniques: combinations of light-, electron-, and force-based ultramicroscopy, experiment and theory. Since plasmonics plays an intimate role in many of these approaches, it will be featured in most of the nine sessions. The sessions will cover videography of molecules captured in real space using ultrafast nonlinear optics from X-rays to THz; nanoscopy and spectromicroscopy in frequency-space domain reaching the Å-limit; space-time resolved dynamics of electrons at interfaces; advances in theory and applications of surface- and tip-enhanced Raman spectroscopy including transport at conductive junctions, cavity optomechanics and light-matter entanglement; plasmon driven chemistry and photophysics including chiroptical response.

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MOLECULAR, ELECTRONIC, AND IONIC TRANSPORT IN MATERIALS FOR ENERGY

Myriad phenomena underlying the transport of ions, small molecules, and electrons drive important properties in self-assembled materials used for energy conversion and storage technologies. Fundamental physicochemical understanding of transport mechanisms will help drive these material systems forward and enable new and efficient applications in energy and sustainability. This symposium will focus on the interplay of multi-scale structure and dynamics on transport, and the influence of molecular features such as collective non-covalent interactions and long-range electronic coupling. Presentations will encompass a range of theoretical and experimental work, with the hope of generating connections among the variety of fields represented as well as building intellectual synergy between the participants.

Louis Madsen, *Virginia Tech*, lmadsen@vt.edu
Xavier Roy, *Columbia University*, xr2114@columbia.edu

COMPUTATIONAL QUANTUM CHEMISTRY: FROM PROMISE TO PROMINENCE *A SYMPOSIUM IN HONOR OF HENRY F. SCHAEFER*

This symposium will celebrate the scientific career of Prof. Henry F. Schaefer III (University of Georgia) by illustrating the evolution of the field of molecular electronic structure (quantum chemistry) from its relatively humble beginnings to its prominent role as a partner to the experiment in chemistry, biology, and materials science. The symposium will provide a retrospective on Prof. Schaefer's leading role in transforming the field to what it is today, as well as highlight the exciting future of quantum chemistry and, broadly, theoretical chemistry. To this end the symposium will bring a mix of senior researchers who will provide perspective on Prof. Schaefer's early work, prominent mid-career researchers responsible for the dramatic recent advances of the field, and bright young stars who will be shaping the field's future.

Edward Valeev, *Virginia Tech,* valeev76@vt.edu
T. Daniel Crawford, *Virginia Tech & MolSSI*, crawdad@vt.edu
C. David Sherrill, *Georgia Tech*, sherrill@gatech.edu
Peter R. Schreiner, *Justus Liebig University Giessen, Germany*, prs@uni-giessen.de

YOUNG INVESTIGATOR RESEARCH AWARDS

Our PHYS Division Young Investigator Research Award talks will be presented during the relevant PHYS technical symposia. **See http://phys-acs.org/postdocs/announce_2019.html**

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session to be held on Wednesday (28 August), from 6:00 to 8:00 PM. Up to six awards with monetary prizes will be given for exemplary work. 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.

On-Line Abstract Submission Deadline: 18 MARCH 2019 **http://abstracts.acs.org**

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