ACS DIVISION OF PHYSICAL CHEMISTRY
256TH NATIONAL MEETING

Boston MA ☛ 19-23 August 2018

Meeting Theme: Nanoscience, Nanotechnology & Beyond

CALL FOR PAPERS

The Division of Physical Chemistry has organized the following topical oral symposia, consisting of both invited and contributed papers. **The abstract submission window opens 15 January and closes on 12 March 2018**. For those interested in an oral presentation, submit abstracts to the appropriate symposium via the ACS MAPS system. 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.

MATERIALS IN EXTREME ENVIRONMENTS

The Symposium will target materials phases emerging in, or retained under extreme conditions, such as extreme pressures, temperatures, or subject to deformations, point impact, and radiation. Such materials are fundamentally intriguing, and also of high importance to areas of technology such as manufacturing of tools, armor, and spacecraft, and also to geochemistry or planetary science. New chemical bonding rules may be necessary under extreme conditions. For example, there can be huge Pauli repulsion, orbital order switching, increased relativistic effects, and prevalence of excited states and/or internal conversion events. The development and use of state-of-the-art experimental and theoretical methods to discover and probe these new phases will be emphasized.

Eva Zurek, *University at Buffalo, SUNY*, ezurek@buffalo.edu
Anastassia N. Alexandrova, *University of California, Los Angeles*, ana@chem.ucla.edu

CHEMICAL APPLICATIONS OF ULTRAFAST X-RAY/XUV SPECTROSCOPY & SCATTERING

Free-electron lasers and high-harmonic sources provide femtosecond to attosecond probes of short-lived states in molecules and materials. Core-level spectroscopy in the x-ray and extreme ultraviolet spectral regions reveals element-specific electron dynamics, while x-ray scattering probes ultrafast structural changes. This symposium will highlight advances in these light sources and the new science they enable. Topics will include catalytic reaction mechanisms in small molecules and proteins, transition metal photophysics, and solar energy conversion.

Josh Vura-Weis, *University of Illinois at Urbana-Champaign,* vuraweis@illinois.edu
Renske van der Veen, *University of Illinois at Urbana-Champaign,* renske@illinois.edu
Philippe Wernet, *Helmholtz Zentrum Berlin,* wernet@helmholtz-berlin.de

STRONG FIELD CHEMISTRY

Laser fields with intensities higher than 10^{13} W/cm^2 interact strongly with the electrons in atoms and molecules. Such interaction results in some interesting and significant physical processes such as above threshold ionization/dissociation and attosecond pulse production (high harmonic generation). While the fundamentals of strong field ionization of atoms itself remains an active research subject, the studies of molecules in a strong field, *i. e.* strong field chemistry, have already attracted much attention due to the added complexity that might reveal new dimensions of strong field dynamics and a potential control approach of chemical reaction afforded by non-perturbative methods. This symposium will bring together scientists who are actively working on the frontiers of strong field chemistry with the goal of providing a platform for communication between experiment and theory.

Wen Li, *Wayne State University*, wli@chem.wayne.edu
H. Bernhard Schlegel, *Wayne State University*, hbs@chem.wayne.edu

ELECTROCHEMICAL INTERFACES

Electrochemical interfaces are ubiquitous in nature and are present in a variety of energy storage technologies—from batteries to double-layer capacitors. Their understanding is challenging experimentally and computationally due to their complex and interdisciplinary nature. This symposium will provide a discussion platform for modeling scientists and experimentalists to exchange ideas on developing novel methodologies and application of existing methods to advance understanding of the structural properties, electrochemical reactions, transport processes under applied electric field at interfaces, as well as how these processes are coupled together. Both modeling and experimental studies are solicited. Primarily focus will be on the charge, mass transport, electrochemical stability and reactions in batteries and electric double layer capacitors; improvement of energy, power density and cycle life of batteries containing liquid or solid electrolytes; and papers dealing with the fundamental aspects of electrochemical interfaces.

Oleg A. Borodin, *US Army Research Laboratory*, oleg.a.borodin.civ@mail.mil
Gleb Yushin, *Georgia Tech*, yushin@gatech.edu
Lamartine Meda, *Xavier University of Louisiana,* lmeda@xula.edu

NEW SPECTROSCOPIC TECHNIQUES FOR ASTROCHEMISTRY

Spectroscopy is the driving force behind astrochemistry, enabling the robust identification of over 200 molecules in the interstellar medium and in circumstellar shells to date. The availability of powerful astronomical facilities like ALMA and SOFIA, as well as the upcoming launch of JWST, continue to provide new opportunities for understanding the chemistry at play in the interstellar medium, star-forming regions, protoplanetary disks, exoplanet atmospheres, and evolved stars. Rigorous laboratory spectroscopy is essential for converting these astronomical observations into scientific insight. In this symposium, we will focus primarily on the development and improvement of spectroscopic tools in the laboratory that will meet the data needs of astrochemistry for the next 10 years—from the radio to the UV, condensed phase to gas phase. We also welcome talks from observers, theorists, and modelers that highlight key data needs for astrochemistry that can be addressed by laboratory spectroscopy.

Kyle N. Crabtree, *University of California, Davis*, kncrabtree@ucdavis.edu
Michael C. McCarthy, *Harvard-Smithsonian Center for Astrophysics*, mmccarthy@cfa.harvard.edu

INFORMATION THEORY AND DYNAMICS: FROM ELEMENTARY PROCESSES TO SYSTEM CHEMISTRY, IN HONOR OF RAPHY LEVINE'S 80TH BIRTHDAY

The development and application of information theory in chemistry has progressed in several directions, from early work on developing an information theoretic approach to molecular dynamics, the so-called surprisal analysis, which describes the interacting molecular systems far from equilibrium to quantum chemistry of optimizing basis sets and describing correlations, to analytical chemistry for the search for a higher selectivity, and efficiency of analytical methods. Recently quantum information theory played a major role of developing techniques and quantum computers to solve important problems in chemistry—particularly focusing on energy transport in light harvesting complexes from the point of view of open quantum systems, entanglement and quantum process tomography. This symposium will highlight invited talks by theoretical chemists and system chemistry pioneers whose work builds on fundamental foundations to describe increasingly complex application of classical and quantum information theory in chemistry.

Sabre Kais, *Purdue University*, kais@purdue.edu
Todd Martinez, *Stanford University*, toddjmartinez@gmail.com

FROM POTENTIAL ENERGY SURFACES TO DYNAMICS AND KINETICS: A PRIORI THEORIES FOR COMBUSTION, ATMOSPHERIC AND INTERSTELLAR CHEMISTRY

This symposium highlights advances in the development of first-principles theoretical approaches for characterizing chemistry in the gas phase and beyond. The coupling of high-level ab initio-based potential energy surfaces with increasingly detailed dynamical models is enabling theoretical predictions with unprecedented accuracy. The increased role of theory as an independent source of quantitative chemical and physical information, along with the approaching age of exascale computing, is anticipated to have a transformative effect throughout chemistry. Themed topical sessions are dedicated to electronic structure methods and potential energy surface development, dynamics and kinetics methodologies, and demonstrations of the impact of a priori theories in combustion, atmospheric, and interstellar chemistry.

Richard Dawes, *Missouri University of Science and Technology*, dawesr@mst.edu
Ahren Jasper, *Argonne National Laboratory,* ajasper@anl.gov

STRUCTURAL PHOTONICS: DETERMINING THE STRUCTURAL INFLUENCE ON THE PHYSICAL PROPERTIES OF PHOTONIC MATERIALS

Photonic materials have outstanding potential to serve as functional components in many applications including catalysis, applied spectroscopy, national security, energy conversion and management, and medical diagnostics and therapeutics. However, achieving these objectives requires predictive descriptions of how nanoscale structure influences the physical properties of these materials. In order to achieve these goals, an intellectual framework that combines fabrication, measurement, and modeling is needed. This symposium will bring together a synergistic group of scientists engaged in describing the structure-dependent physical properties of photonic materials. We will discuss the composition-structure-function interplay for novel systems composed of plasmon-supporting and semiconducting materials. Emerging photonics materials will be a major focus, including 2D and layered materials, and the challenges of establishing systems based on inexpensive and earth-abundant precursors. Recent experimental and computational advances for characterizing and predicting new materials and structures will be explored in depth. Sessions will focus on the state-of-the-art in structurally precise material fabrication, experimental characterization techniques, and computational modeling.

Kenneth L. Knappenberger, Jr., *Penn State University,* klk260@psu.edu
A. Eugene DePrince, *Florida State University,* deprince@chem.fsu.edu
Adam Schwartzberg, *Lawrence Berkeley National Lab,* ams@lbl.gov

CHARACTERIZATION, DETECTION, AND APPLICATION OF EXCITONS IN CHEMISTRY

An exciton is a fundamentally quantum mechanical object created when a photon is absorbed by an aggregate of chromophores. This aggregate can take the form of a molecular assembly, an inorganic semiconductor, or a group of pigments embedded in other environments. Excitons serve as the active players in diverse optoelectronic processes like solar light harvesting, optical imaging, lasing, and sensing. Despite a long history of research dating back to the early days of quantum mechanics, the classification and quantitative description of excitons have remained difficult challenges in physical chemistry. This is particularly true in the intermediate regime between the well-known limits of Frenkel and Wannier excitons. The study of excitons has gained a new urgency due to the development of new solar energy materials (e.g. perovskites) and the observation of new phenomena like multiple exciton generation and exciton fission, motivating recent advances in computational modeling and spectroscopic detection of the spatio-temporal dynamics of excitons. This symposium will bring together a diverse group of theoretical and experimental researchers working on the characterization, detection, and application of excitons in organic, inorganic, and biological materials. The objective is to facilitate discussion among these different groups, to develop consensus on how to measure and classify excitonic phenomena, and to identify new and promising directions of future research.

Seogjoo J. Jang, *City University of New York – Queens College*, sjang@qc.cuny.edu
Christopher J. Bardeen, *University of California, Riverside*, christob@ucr.edu

SYMPOSIUM IN MEMORY OF AHMED ZEWAIL: ULTRAFAST MOLECULAR SCIENCES BY FEMTOSECOND PHOTONS AND ELECTRONS

This special symposium in memory of the late Ahmed Zewail will include invited and contributed talks on the most recent advances in Femtoscience, including theory and experiments. Topics will include reaction dynamics in gas, liquid, and at interfaces, charge transfer processes, primary processes in biology, and electron dynamics with ultrafast diffraction and imaging. These studies are now possible, thanks to developments in mid-IR, Vis, UV, X-Ray, and electron pulses with durations on the femtosecond and attosecond timescales, many of which were pioneered by Ahmed Zewail.

Dongping Zhong, *The Ohio State University*, zhong.28@osu.edu
Marcos Dantus, *Michigan State University*, dantus@chemistry.msu.edu

PHYS DIVISION RESEARCH AWARDS AND PHYS/JPC LECTURESHIP AWARDS

The four winners of the PHYS Division Research Awards and the three winners of the PHYS/Journal of Physical Chemistry Lectureship Awards will present talks at this half-day symposium on Aug 21st.

PHYSICAL CHEMISTRY SYMPOSIUM WORKSHOP FOR UNDERGRADUATE CHEM MAJORS

The Workshop for Undergraduate Chemistry Majors is designed 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/2018.html. The application deadline is **26 February 2018**.

Casey Londergan, *Haverford College*, ug-phys@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, 22 August 2018. See announcement below for information about the Physical Chemistry Student Poster Awards.

On-Line Abstract Submission Deadline: 12 March 2018 **http://abstracts.acs.org**

YOUNG INVESTIGATOR RESEARCH AWARDS (formerly the PHYS Postdoc Awards)

Four PHYS Division Young Investigator Research Award talks will be presented during the relevant PHYS technical symposia**.** See http://phys-acs.org/postdocs/announce_2018.html

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.

MICHAEL A. DUNCAN, PROGRAM CHAIR **University of Georgia (706) 542-1998, maduncan@uga.edu**

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