CALL FOR PAPERS

ACS DIVISION OF PHYSICAL CHEMISTRY
SPRING 2023 NATIONAL ACS MEETING
"Crossroads of Chemistry"
Indianapolis, Indiana ☺ 26 - 30 March 2023

The Division of Physical Chemistry (PHYS) is hosting the following nine oral symposia, consisting of both invited and contributed papers, as well as a general poster session. **Abstract submission will open on August 15 and remain open until October 17**. For those interested in an oral presentation, please submit abstracts to the appropriate symposium via ACS-MAPS. 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.

Peter G. Wolynes 70th Birthday Symposium

Peter Wolynes, the D.R. Bullard-Welch Foundation Professor of Science and Professor of Chemistry at Rice University, is a world-renowned leading scientist and inspirational role model. Prof. Wolynes' pioneering work, with its numerous brilliant and piercing insights, has changed the thinking and direction of modern experimental, theoretical, and computational research in many different fields, including protein folding and dynamics, the glass transition, and reaction dynamics, among others. Covering an unprecedented range of topics, his research has a unifying theme, that of many-body physics emerging in complex free energy landscapes. In the spirit and recognition of Prof. Wolynes' work, this symposium will bring together theorists and experimentalists covering a wide range of research topics.

David Leitner, *University of Nevada, Reno*, dml@unr.edu
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Experimental and Theoretical Progress in Multidimensional Spectroscopy: Elucidating Charge and Energy Transfer in the Condensed Phase

Understanding and controlling the abilities of materials, such as molecular aggregates, solvated chromophores, and nanomaterials to hold, transport, and guide energy is critical for next generation photocatalysts and energy conversion and storage technologies. Recent advances in multidimensional spectroscopies (such as two-dimensional electronic-vibrational spectroscopy and ultrafast X-ray-optical spectroscopies) have made it possible to capture excitation dynamics in a wide variety of materials with unprecedented spatial and temporal resolution. However, interpreting these spectra remains a formidable challenge. To address this knowledge gap and provide a fully first-principles approach to modeling excited-state processes in the condensed phase, recently developed theoretical methods aim to capture important components of the problem, including couplings to nuclear motion, environmental polarization effects, and couplings between different excited states. In this symposium, experimentalists and theorists will have the opportunity to present recent developments in novel multidimensional spectroscopies and the methods necessary to simulate, interpret, and predict these measurements.

Tim J. Zuehlsdorff, *Oregon State University*, zuehlsdt@oregonstate.edu
Andrés Montoya-Castillo, *University of Colorado*, andres.montoyacastillo@colorado.edu
David Coker, *Boston University*, coker@bu.edu

Innovative Teaching in Physical Chemistry

Undergraduate physical chemistry education spans a wide range of topics from traditional areas such as thermodynamics, kinetics, and quantum mechanics to advanced and emerging topics such as statistical mechanics, computational chemistry, spectroscopy, and advanced instrumentation. This session focuses on innovative curricula, activities, and best practices for teaching undergraduate physical chemistry courses, including both lecture and laboratory courses. We particularly encourage submissions that discuss active learning pedagogies in physical chemistry including, but not limited to, course-based undergraduate research experiences (CUREs), team-based learning, inquiry-based learning, and project-based learning. We also welcome activities that focus on data literacy including programming, data analysis, data visualization, and data science in chemistry. Submissions may discuss a particular activity for teaching physical chemistry or larger course- or program-level curricular innovations.

Ashley Ringer McDonald, *Cal Poly San Luis Obispo*, armcdona@calpoly.edu
Elizabeth Thrall, *Fordham University*, ethrall@fordham.edu
Grace Stokes, *Santa Clara University*, gstokes@scu.edu
Mark Hendricks, *Whitman College*, hendrimp@whitman.edu

Frontiers of Structural Biology in Complex Environments

Decades of careful experimentation and analysis by biophysical chemists have formed a foundation for contemporary scientists to understand the structure and function of proteins in the incredibly complex environments of living organisms. Recent advances in experimental and computational approaches have made it possible to describe and predict the structure, dynamics, and interactions of biomolecular assemblies in complex environments in vitro, in situ, in cells, and in the extracellular environment. Despite these exciting advances, many challenges remain in integrating techniques and approaches that span multiple time and length scales, and in understanding how atomic level changes drive functional biological outputs in the cellular environment. The symposium will bring together experimentalists and theorists who apply cutting-edge methods to determine the structure of biomolecules at or near atomic level precision in such environments. Speakers will discuss recent progress in the field and future challenges in the areas (1) atomic resolution studies of large complexes, (2) biomolecular condensation, (3) in situ studies in cell and cell-like environments, (4) in vitro cellular environments, and (5) biophysical experiments in multi-cellular environments.

Matthew Eddy, *University of Florida*, matthew.eddy@chem.ufl.edu
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Bridging the Gap: Using Gas-Phase and Cluster Studies to Model the Dynamics of Complex Systems

The traditional methods of physical chemistry can unravel intricate details of chemical structure and dynamics, but applying these tools to important problems in complex, condensed-phase, and strongly interacting systems remains a challenging frontier. Pioneering experimental and theoretical work continues to expand our toolkit, enabling careful interrogation and interpretation of molecular dynamics and photoinduced processes in environments of increasing complexity. Gas-phase and cluster model systems remain invaluable as platforms for detailed experimental and theoretical studies to unravel key aspects of complex processes in such diverse fields as atmospheric and aerosol chemistry, astrochemistry, nonadiabatic dynamics, ultrafast photophysics, and energy sciences. This symposium will identify new challenges and directions in molecular dynamics and photochemistry for which gas-phase and cluster studies can have significant impact. We aim to bring together leading experts as well as early-career investigators beginning new work to stimulate discussion and foster collaborations spanning experiment and theory.

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Charge Transfer and Energy Conversion at Interfaces and Defects

Many emergent technologies rely on understanding the dynamics of charge and energy transfer in materials. Some examples include solar energy conversion in molecular and solid-state systems, plasmon-driven chemistry, and spin-processes. Heterogeneities such as interfaces and defects have a large impact on such dynamics, resulting in both desirable and undesirable outcomes. With the advancement of computational & experimental techniques, new insight into these excited-state processes can be gained at short (fs) time scales and on the atomic scale, and directly connecting simulation to experiment in materials whose properties are determined by defects and/or interfaces remains a significant challenge. This symposium will bring together computational and experimental researchers in the field of charge transfer and energy conversion in nanostructured materials, with a focus on defects and interfaces, and emerging phenomena in this field, such as strong couplings between light and matter and spin processes. The emphasis will be on new theoretical and computational methods developments, the applications of simulation to real-world problems, and cutting-edge experiments that drive the need for advances in theory.

Pengfei (Frank) Huo, *University of Rochester*, huo@chem.rochester.edu
Benjamin G. Levine, *Stony Brook University*, ben.levine@stonybrook.edu
Sahar Sharifzadeh, *Boston University*, ssharifz@bu.edu

Carbon Separation and Capture at the Atomistic Level: Theory and Experiment

The increasing concentration of CO_2 is impacting environmental degradation—notably in higher global temperatures, rising sea levels, increased ocean acidity, and more extreme weather-related events. This symposium will bring together computational and experimental researchers who are actively exploring the physicochemical effects at the atomistic level that govern carbon separation and capture processes. This symposium will cover technologies that are based, among others, on direct air capture, biomimetic processes, ionic liquids, porous materials, and polymeric membranes. Contributions from diverse and interdisciplinary research areas such as spectroscopy, simulations, data sciences, synthetic chemistry, materials science, and engineering are invited. The key role of intermolecular interactions of CO_2 with functional units of amorphous or crystalline materials at both experimental and theoretical level will be a central topic in the symposium.

Sheng Dai, *Oak Ridge National Laboratory*, dais@ornl.gov
Konstantinos D. Vogiatzis, *University of Tennessee, Knoxville*, kvogiatz@utk.edu

New Directions in the Physical Chemistry of Organic Semiconductors

To date, progress in the field of organic semiconductors (OSCs) has been largely driven by intense interest in organic photovoltaics, field-effect transistors, and light-emitting diodes. However, new research directions have emerged beyond such classical applications, such as mixed electronic/ionic conductors, thermoelectrics, highly doped materials and stretchable/flexible thin films. These developments have uncovered new knowledge gaps that have risen to the forefront of the evolving OSC field. Questions about the coupling between electronic and ionic degrees of freedom, the influence of microstructure on mechanical properties, and quasiparticle transport in complex environments demand further attention. This symposium will highlight new directions in OSC materials research in both small molecules and polymers. The organizers will bring together experimental, theoretical, and computational communities to address current knowledge gaps and catalyze discovery of new ones in the design, construction and performance of OSCs.

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Benjamin J. Schwartz, *University of California, Los Angeles*, schwartz@chem.ucla.edu

The Physical Chemistry of Co-translational Protein Folding

Protein folding has long been interpreted through the lens of in vitro refolding experiments on small proteins that conform to two- (or few) state models, though this may be a poor model for how proteins fold in the cell, which occurs cotranslationally on the ribosome. Translation makes folding an inherently kinetic phenomenon replete with irreversible steps, and may be required for the folding of more complex 'non-model' proteins. This symposium will critically elucidate differences between protein folding in vivo compared to traditional in vitro refolding assays so as to shed light as to where our 'received truths' about protein folding might need to be reconsidered. It will also emphasize the important interplay between computation and novel experimental techniques to elucidate a complex process that is somewhat elusive to traditional methods in biophysical chemistry and structural biology.

Stephen D. Fried, *Johns Hopkins University*, sdfried@jhu.edu
Silvia Cavagnero, *University of Wisconsin*, cavagner@chem.wisc.edu
Edward O'Brien, *Penn State University,* epo2@psu.edu

PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session. Multiple awards 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: OCTOBER 17, 2022 **http://abstracts.acs.org**

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