CALL FOR PAPERS

PHYS Physical Chemistry
ACS Technical Division

ACS DIVISION OF PHYSICAL CHEMISTRY
FALL 2024 NATIONAL MEETING
THEME: ELEVATING CHEMISTRY
AUGUST 18-22, 2024 ◈ DENVER, COLORADO

The Division of Physical Chemistry (PHYS) is hosting the following ten oral symposia, consisting of both invited and contributed papers, as well as a general poster session. **Abstract submission opens January 8 and closes April 1, 2024**. 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.

ELUCIDATING THE CHEMICAL SPECIFICITY OF BIOMOLECULAR CONDENSATES

Biological condensates play essential roles in various cellular processes, from stress response to genome organization. Similar to membrane-bound organelles, they assemble a collection of molecules to raise the efficiency of sophisticated tasks. The lack of a membrane barrier allows fast material exchange between condensates and the cellular environment, rendering the molecular composition and stability of condensates more prone to regulations by external signals. Intrinsically disordered proteins (IDPs) that promote multivalent, promiscuous interactions are key drivers of condensate formation. Multiple mechanisms, including electrostatic, cation-π, hydrogen bonding, and hydrophobic interactions, contribute to the affinity among various chemical groups. Above a threshold concentration, as predicted by the Flory-Huggins theory, interactions among IDPs can drive liquid-liquid phase separation to produce a highly concentrated phase that nevertheless remains dynamic. Despite significant progress, much remains to be learned regarding the connection between amino acid sequences and protein phase behaviors, or the so-called "molecular grammar" of protein condensates. Systematic and quantitative structural and chemical characterizations of condensates are necessary to understand their organizational principles further. This symposium will bring together theorists and experimentalists to present the latest progress in studying biomolecular condensates, identify future challenges, and promote collaborations.

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UNDERSTANDING PROTEIN STRUCTURE WITH SPATIALLY AND TEMPORALLY RESOLVED SPECTROSCOPY

At the heart of many fundamental biological and pathological processes is the transformation and evolution of specific structures by protein and peptide assemblies. A persistent experimental challenge is the development of biophysical approaches that offer new insights into protein conformation and dynamics. Application of ultrafast time-resolved spectroscopies has led to successful experimental designs that leverage the nonlinearity of protein signals and provide site-specific structural constraints, akin to nuclear magnetic resonance spectroscopy. More recent advances have augmented molecular spectroscopies with spatially-resolved imaging techniques, revealing individual structures within an ensemble. The advent of cryoelectron microscopy has furthered the potential of spatially-resolved structural mapping of biomolecular self-assemblies. Altogether, these approaches probe protein structure with unprecedented detail. This symposium will bring together experts in imaging, spectroscopic, and computational methods, and we encourage invited speakers to frame their talks with respect to recent advances and future challenges for the field, in the hopes of spurring conversations and collaborations that will advance our understanding of how protein structures evolve related to both biological function and pathological consequences.

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NEW METHODS AND APPLICATIONS OF RAMAN SPECTROSCOPY AND MICROSCOPY

In the recent past, experimental physical chemists have greatly expanded the utility of methods based on Raman scattering to explore a vast array of systems. New, innovative, and highly useful spectroscopy and microscopy techniques based on Raman scattering have expanded our ability to probe systems from molecules to materials to living organisms. This symposium will highlight the latest methods—including spectroscopic techniques such as FSRS, single-molecule Raman spectroscopy, methods that enhance Raman signals, and cutting-edge Raman microscopy methods—and the theoretical descriptions and predictions that complement experimental methods. Topics will include: coherent Raman spectroscopy and imaging; SERS and plasmon-enhanced spectroscopy and imaging; non-linear and time-resolved Raman spectroscopy; tip-enhanced Raman spectroscopy (TERS); and advances in commercial Raman instrumentation.

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ADVANCED NANOPARTICLE CHARACTERIZATION

Advances in laboratory- and facility-scale measurement techniques have opened new doors for the quantitative analysis of nanoparticles. This symposium will bring together researchers developing these new capabilities and employing them to solve nanoparticle problems across a range of disciplines from environmental chemistry to catalysis. The technique-forward focus of this symposium is geared toward attracting nanoscience researchers who are unfamiliar with these advanced tools and also cross-pollinating ideas and approaches developed in disparate disciplines—from atmospheric science to catalysis or energy storage—that do not typically feature strong scientific overlap. Approaches to characterizing nanoparticles will include: X-ray techniques, neutrons, vibrational spectroscopy, electronic spectroscopy, magnetic resonance, microscopy, X-ray free electron lasers, and the application of machine learning to these techniques. Topics of interest include atomic structure, electronic structure, structural dynamics, links to function, interfacial interactions, and optical phenomena.

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ENERGY APPLICATIONS OF ULTRAFAST SCIENCE

The optimization of solar energy technologies requires the investigation of the structure and dynamics of solar energy materials and processes across relevant time- and length- scales. Time-resolved techniques have emerged as a significant means of achieving a deep comprehension of the fundamental principles behind photoinduced processes involved in solar energy conversion. This symposium will showcase the most recent breakthroughs facilitated by these innovative scientific approaches. The work presented will encompass a wide range of topics, exploring photoinduced reaction mechanisms across diverse domains such as small molecules, transition metal complexes, nanomaterials, and solid-state materials. This exploration will utilize a variety of time-resolved spectroscopic techniques, spanning from the microwave to the X-ray regime, all of which exhibit tremendous potential for driving and directing efforts toward efficient solar energy conversion. The symposium will include topics like: charge carrier dynamics in semiconductors; molecular photophysics and photochemistry; vibrational/vibronic effects in photochemistry; time-resolved in situ spectroscopy; and photocatalysis and photoredox.

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METHODS AND APPLICATIONS OF SINGLE-MOLECULE DETECTION

Experimental methods that are based on detection, microscopy, and spectroscopy of single molecules have revolutionized the study of topics ranging from biology to materials science to chemical reaction dynamics. The ability to probe single molecules provides a unique window into heterogeneity in complex systems, and the ability to manipulate them provides precise control over folding and reaction pathways and quantum properties. The single-molecule field has made constant advances in the measurement capabilities of instruments, the sophistication of data analysis and modeling techniques, and the breadth and depth of applications. This symposium will communicate advances in methods and applications of single-molecule detection, microscopy, and spectroscopy, to a broad audience. Sessions focused on methods will report advances in instrumentation, modeling and data analysis. Additional sessions will be devoted to cutting-edge applications of single-molecule methods to problems in biology, sensing, materials science and catalysis. The work presented in this symposium will be of value to all researchers with an interest in these subject areas and all who utilize single-molecule methods for various applications.

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LATTICE DYNAMICS: CHARACTERIZATION AND APPLICATIONS

Crystal lattice dynamics impact a wide range of bulk physical properties, ranging from thermal expansion to superconductivity. While the relationship between lattice structure and crystal properties is well-established, the role of specific vibrational motions on crucial condensed phase properties—including phase transformations, mechanical and thermomechanical responses, charge carrier dynamics, and gas adsorption in porous crystals—has only recently been uncovered, opening new and exciting areas of research. The dynamic lattice plays a profound role in dictating both the equilibrium properties of materials as well as their response to external stimuli. Lattice dynamics are inherently broadly defined, occurring across a large frequency range and involving a variety of vibrational modes that are often interconnected. This complexity requires new experimental tools to probe dynamics. From a theoretical perspective, there exist significant opportunities to understand the properties of crystals through the lens of atomic and molecular dynamics. This symposium will feature cutting-edge research of broad general and technological interest and aims to highlight recent advances and areas for interdisciplinary studies—ranging from crystal growth and design to characterization and applications.

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ENHANCED SAMPLING METHODS FOR THE STUDY OF CHEMICAL REACTIONS AND CONFORMATIONAL TRANSITIONS

The computational study of the dynamics of chemical reactions and conformational transition has undergone a true revolution in the past 20-30 years. While quantum chemistry approaches that allow one to find potential energies along specific reaction coordinates have existed for far longer, the ability to follow the rare event of a chemical reaction has remained a significant challenge that is only now being met through the development and application of a variety of enhanced sampling methods. These methods not only allow the observation of long-timescale events; in many cases, they also allow for the computation of rigorous statistical mechanical data. This symposium will gather experts who will describe both methodological developments and applications to problems of real chemical interest. This symposium will feature speakers developing a range of cutting-edge computational approaches, including multi-tempering simulations, collective variable methods, replica exchange, accelerated MD, transition path and transition interface sampling, milestoning, and the use of machine learning methods for collective variable identification. The applications are expected to range from gas-phase chemical reactions to modeling of materials and complex biological systems.

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Steven Schwartz | University of Arizona | sschwartz@arizona.edu
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OPEN-SOURCE SOFTWARE IN PHYSICAL CHEMISTRY

This Convergent Research Community (CRC) Innovative Project Grant symposium will focus on open-source software in physical chemistry and is complemented by other open-source software symposia in the CATL, CINF, and COMP divisions. The emphasis of this PHYS symposium is to bring together experts that focus on 4 core areas: (1) best practices/resources in open-source software development applicable to different physical chemistry research environments (from PUIs to National Laboratories); (2) open-source software in electronic structure theory; (3) open-source software in statistical mechanics and dynamics; and (4) open-source software in machine learning.

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ADDRESSING THE COMPLEXITY OF CORRELATED QUANTUM MANY-BODY PROBLEMS BY EMBEDDING AND DOWNFOLDING

The detailed first-principles description of the ground and excited state electronic structure in molecules and solids is nominally associated with a high, often unsurmountable, computational cost. Practical approaches thus rely on introducing systematic approximations to the quantum many-body interaction terms. The perturbative treatments are limited to systems with weak or moderate electronic correlations. For other cases, the system is partitioned into a correlated subspace with reduced dimensionality, on which the remaining interactions are downfolded. Multiple complementary approaches exist to achieve such a complexity reduction. In recent years, various techniques have been explored and bridged distinct theoretical concepts and research fields. This symposium will feature theorists developing theoretical and computational many-body techniques at the intersection of disciplines, and it will discuss recent progress and challenges, ranging from methodologies for capturing correlation effects to embedding formulations that integrate these methodologies across various scales. This symposium will focus on conceptual and technical advances enabling the treatment of realistic molecular and solid-state systems.

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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/young-investigator-award-phys/ for application information.

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: 1 April 2024 **http://abstracts.acs.org**

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