CALL FOR PAPERS

PHYS Physical Chemistry
ACS Technical Division

ACS DIVISION OF PHYSICAL CHEMISTRY
SPRING 2025 NATIONAL MEETING
MARCH 23-27, 2025
SAN DIEGO, CALIFORNIA

The Division of Physical Chemistry (PHYS) is hosting the following eight oral symposia, consisting of both invited and contributed papers, as well as a general poster session. **Abstract submission will open on August 5 and closes on September 30, 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.

Light-Matter Interactions in Molecular Systems and Emerging Semiconductors

Light-matter interactions are ubiquitous in the world of optoelectronic devices. These interactions have been shown to vary across material family, dimensionality, and composition. Scientists and engineers have been able to utilize these interactions to drive new and exciting science in fields ranging from solar energy conversion and light emission to catalysis or biointeractions. In this symposium, the organizers intend to open a dialog between experimental and computational scientists working to resolve the complex photophysical processes occurring in molecular systems, emerging semiconductors across dimensionalities and material systems, highlighting both the similarities and differences towards a universal understanding of light-matter interactions.

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Frontiers in Coherent Nonlinear Spectroscopy and Hyperspectral Microscopy

Coherent nonlinear optical spectroscopy has been a powerful tool for elucidating the structure and dynamics of molecular, materials and biological systems. The field has witnessed tremendous growth over the past few years, achieving broader spectral range, higher spatial resolution, and enhanced detection of weak signals by the implementation of new light sources, new polarization schemes, and coupling with microscopy. These technical innovations have broadened and deepened our understanding of the ultrafast photophysics of a wide range of systems and their functions microscopic and macroscopic length scales and many degrees of freedom. This symposium aims to bring together domestic and international experimentalists at the forefront of both methodology development and application of coherent nonlinear spectroscopy and hyperspectral microscopy for understanding the spatiotemporal dynamics of molecular, biological, and materials systems.

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QIS for Chemistry and Chemistry for QIS

This symposium is designed to stimulate provocative discussions on big questions at the interface between quantum information science and chemistry. From spin qubits to trapped ions, chemical principles such as bonding, reactivity, and symmetry play a critical role in building complexity and optimizing novel quantum systems. However, chemistry is a relatively new participant in the QIS field, owing to previous difficulties in combining molecular complexity with the necessity for “clean” state preparation and measurement. This symposium will bring in researchers who are working at this interface, with the aim to discuss paths which allow for routine design and discovery of new QIS compatible systems. We are particularly motivated by areas where QIS can be applied to probe chemical change, and areas where chemical intuition can be brought to optimize or add functionality to existing QIS systems.

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Inferring Kinetics, Thermodynamics, and Mechanisms from Enhanced Sampling Simulations

Enhanced sampling techniques can offer far-reaching capabilities beyond merely exploring molecular configurational space. If the proper tools are developed, they can provide a profound understanding of molecular mechanisms at the atomic level, facilitate precise determination of thermodynamic properties from a statistical standpoint, and enable inference of rates and kinetics associated with complex molecular processes. Several exciting developments have recently been reported that address these three topics precisely. A very partial list of examples includes using Boltzmann generators or other advanced machine-learning algorithms for sampling equilibrium distributions; employing stochastic resetting, normalizing flows, or Kramers theory for improved kinetics inference; and employing enhanced sampling techniques for understanding the mechanisms of supramolecular self-assembly, or perovskite nucleation. This symposium aims to convene experts in the field to delve into recent advancements, facilitate knowledge exchange, and chart a trajectory of future developments.

Barak Hirshberg	Tel Aviv University	hirshb@tauex.tau.ac.il
Giovanni Maria Piccini	Universita degli Studi di Modena e Reggio Emilia	piccini@unimore.it

Reactivity in Microdroplets: Challenges and Potentials

Evidence shows that both the kinetics and thermodynamics of reactions in microdroplets can be vastly different from bulk. In many cases either acceleration or deceleration of reaction rates of up to six orders of magnitude have been reported. Despite many successes in this field, the origin and mechanistic details of microdroplet chemistry is still hotly debated. This symposium brings together theoreticians and experimentalists with a diverse range of expertise to catalyze further understanding in this field.

Microdroplet chemistry is relevant to a number of contemporary fundamental and applied problems. It holds potential for scaled up synthesis of pharmaceuticals. It has been implicated as a possibility in the synthesis of pre-biotic molecules. It is known to be relevant to atmospheric reactions. It is a truly interdisciplinary topic, spanning the divisions of physical chemistry, analytical chemistry, organic chemistry, and atmospheric chemistry.

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Electrolytes at Charged and Metallic Surfaces

Meeting current world energy demands with renewable and sustainable energy sources requires efficient energy conversion and storage technologies. Of particular interest are electrochemical technologies, such as electrocatalysis, fuel cells, and batteries. At the heart of these technologies are interfaces where electrolyte solutions meet electrode surfaces, and their knowledge-based control and creation requires a molecular-scale understanding of the complex physical chemistry of the electrical double layer that results at such interfaces. This symposium will focus on the physical chemistry of liquid and solid electrolytes in contact with electrodes and other charged surfaces from a variety of theoretical and experimental perspectives that span a wide range of length and time scales. We encourage contributions that focus on the chemistry of interfaces, as well as relevant investigations on the physical chemistry of electrode and electrolyte materials. The symposium will bring together ultrafast spectroscopists, NMR spectroscopists, electrochemists, materials chemists, computational and theoretical chemists, and more, showcasing a variety of perspectives and encouraging synergy among diverse perspectives.

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A Symposium to Honor Eric Herbst’s Contributions to Our Understanding of the Molecular Universe

Anyone who has worked in the field of astrochemistry will have come across Eric Herbst. Eric Herbst changed our understanding of the reactivity of molecules in the interstellar medium. He showed that interstellar molecules are not just chemists’ curiosities but are excellent probes of physical conditions. His influence has been felt through his mentorship and generous collaborations and the current field is populated with his former students and postdocs, now leading their own research groups in astrochemistry.

This symposium will honor Eric Herbst's immense contributions to the field, upon his retirement, by bringing together his former students, postdocs and collaborators from across the globe to discuss current state of the art and future directions in astrochemistry.

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Computational & Theoretical Modeling of Biomolecular Dynamics in Crowded Environments

This symposium focuses on computer simulations and theory that pivots away from description of individual biomolecules in dilute solution towards systems that are strongly perturbed by interactions between biomolecules. This includes most physiologically relevant environments such as the cytoplasm and membranes of living cells as well as the conditions in condensate droplets formed during liquid-liquid phase separation.

Modeling systems of such complexity is a long-standing challenge for molecular simulations due to the vast number of particles required to capture their complexity with simultaneously increasing timescales required to sample properties and relevant dynamic processes. Current approaches range from computationally expensive all-atom models to highly coarse-grained patchy particle simulations as well as multiscale simulations that combine simulation models with varying resolution.

In recent years, the field has benefitted from increasingly available experimental data on biomolecular properties in living cells and other crowded environments such as liquid condensates, drastically increasing availability of high-performance computing infrastructure as well as the rise of machine learning applications that can provide a bridge between distinct resolutions in multiscale simulations.

This symposium will highlight these advances and the diversity of computational and theoretical researchers in the field. Our program will focus on distinct aspects of biomolecular interactions in simulations, ranging from a) protein-protein binding and complex assembly; to b) biomolecular condensation and molecular crowding in physiological conditions; c) simulations of very large systems with methods ranging from all-atom molecular dynamics, Brownian dynamics and Monte Carlo; and d) multiscale modeling with and without invocation of machine learning tools.

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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: 30 September 2024 **http://abstracts.acs.org**

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