CALL FOR PAPERS

PHYS Physical Chemistry
ACS Technical Division

ACS DIVISION OF PHYSICAL CHEMISTRY
SPRING 2024 NATIONAL MEETING
THEME: MANY FLAVORS OF CHEMISTRY
MARCH 17-21 2024 ◈ NEW ORLEANS, LOUISIANA

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 will open on August 7 and closes on October 2, 2023**. 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.

Informed Design of Quantum Dots and Quantum Dot Assemblies for Energy Applications

The design of quantum dot-based platforms for energy conversion, energy storage, or energy-efficient lighting is predicated on a deep understanding of the photophysical properties of quantum dots (QDs) as a function of their intrinsic characteristics (size, composition, shape) as well as extrinsic factors (surface/interfacial chemistry, component integration). While experimental and computational studies have led to considerable progress in understanding the intrinsic behavior of simple QDs, there is an urgent need to better understand how QDs interact with one another, with the environment, and with other functional components in order to design systems for energy conversion and related applications. This symposium will highlight how experimental and computational insights into QD chemistry and physics enable the design of functional structures based on just one QD or many. Topics will include photon and carrier dynamics in QDs and QD assemblies; tuning the energy landscape via surface or interfacial control; and design of photocatalysts, solar cells, and LEDs.

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Recent Progress in Theoretical Methods for Coupled Quantum Systems

While quantum chemistry is most focused on describing electrons, it is often important in chemical systems to describe non-electronic degrees of freedom such as nuclei, photons, or phonons using quantum mechanics. For many of these systems, it is also essential to include accurate couplings between these degrees of freedom and the electrons. Examples of chemical phenomena where such couplings can be important include (1) nuclear-electronic dynamics and vibronic coupling; (2) polaritonic chemistry such as cavity quantum electrodynamics; and (3) electron-phonon couplings that affect the transport and thermodynamic properties of solids. Numerous theoretical methods to describe these phenomena have been developed. Despite the underlying similarities of the methods, which all treat non-electronic degrees of freedom quantum mechanically while coupling them to the electronic degrees of freedom, theoretical developments and researchers in different fields often remain isolated from one another. The goal of this symposium is to bring these different theoretical fields together for an exchange of ideas, which will lead to collaboration and cross-fertilization among fields. A joint session on polaritons will be held together with the "Current Trends in Polariton Chemistry" symposium.

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Current Trends in Polariton Chemistry

Growing interest in modifications of chemical properties induced by coupling molecular excitations and optical cavities, surface phonon-polaritons, and plasmon-polaritons has produced a broad range of studies on the spectroscopy, kinetics, and thermodynamics of hybrid light-matter systems. However, the relevance of several important polariton characteristics including the collective nature of strong light-matter coupling, the role of classical and quantum mechanical phenomena, and the reproducibility of key experimental findings remain open issues. This symposium will enable direct and critical communication between experimental, computational, and theoretical researchers working at different limits of polariton formation, characterization, and phenomenology to address these issues. This communication will help this fast-growing community better understand how to adequately compare and model similar, yet fundamentally differing results across material and photonic platforms. The resulting advanced understanding will enable the polariton research community to accurately determine and predict the properties of molecular polaritons central to their ability to impact the future of chemical science. A joint session on theory will be held together with the "Recent Progress in Theoretical Methods for Coupled Quantum Systems" symposium.

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Liquid and Electrolyte Anomalies in Nano-Confinement: Structure, Dynamics, and Reactivity

Confinement effects in water-filled inorganic nanopores have cross-cutting significance for water treatment, catalysis, separations, energy storage, corrosion/degradation, and environmental sciences. Nanoconfinement of liquids leads to anomalous behaviors including fast ion transport, higher proton mobility, higher gas solubility, and lower dielectric constants. The enhanced electrostatic interactions, modified acid-base behaviors, and peculiar hydrogen bonding structures pose challenges to traditional theories/approaches. Experimental techniques used to elucidate reactivity and dynamical processes are rapidly developing; however, universal theoretical scaling relationships for reactivities, capacitance, ion-pairing, ion-ion interactions, and associated thermodynamic and kinetic properties remain to be established, especially at finite salt concentrations. We postulate that ion solvation free energies constitute a key descriptor, and that dielectric responses provide a unifying framework for predicting reactivities in water-filled nanopores. This symposium focuses on recent advances describing the structural/dielectric properties, kinetics of reaction and transport, and equilibrium states in inorganic nanopores developed by chemists, physicists, and geochemists to highlight emerging/synergistic research. It discusses future interdisciplinary research opportunities to illuminate nanoconfinement-driven changes to the physico-chemical properties of water which govern speciation, reaction rates, pathways, and products in nanopores.

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Innovative Teaching in Physical and Computational Chemistry

The current undergraduate physical chemistry curriculum has developed to span a wide range of topics. The traditional topics of thermodynamics, kinetics, and quantum mechanics have spawned a more intensive exploration of advanced and emerging topics such as statistical mechanics, computational chemistry, spectroscopy, and advanced instrumentation. This symposium focuses on innovation in curriculum, activities, and best practices for teaching undergraduate physical, computational, and biophysical chemistry courses technically and creatively. This includes 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 (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.

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In Honor of Gregory Voth's 65th Birthday: From Quantum Dynamics to Ultra Coarse-Graining, and Everything in Between

This symposium will celebrate Gregory Voth's impact on the field of physical chemistry on the occasion of his 65th birthday. Over the course of his career, Voth has made seminal contributions to the development of theoretical and computational methodologies to further our understanding of important chemical and biophysical processes. This exciting symposium will bring a combination of both theoretical and experimental researchers to present cutting-edge research over a wide range of topics influenced by his work. These topics will span recent developments in theoretical and computational chemistry such as multiscale modeling, including ultra-coarse-graining, and quantum dynamics as well as interesting problems relevant to chemistry, biochemistry, biophysics, and materials science (e.g., energy storage materials).

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Vibrational Dynamics: Spectroscopy and Imaging

The fast dynamic and structural information uncovered by two-dimensional and one-dimensional vibrational spectroscopy and imaging has benefited our understanding of fundamental molecular insights in biological and material science systems as well as in a wide variety of other disciplines. While advances in experimental developments and theoretical approaches have each made contributions to vibrational spectroscopy and imaging, the combined efforts from both sides have driven and will continue to push the boundaries of vibrational techniques that neither approach can achieve alone. This symposium will bring together experimental, computational, and theoretical scientists in the fields of vibrational spectroscopy and imaging to discuss issues central to these techniques to solve chemical problems. It aims to stimulate discussion between experimentalists and theorists to synergize their efforts to investigate complex problems.

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Chemistry of Ice

Water ice is one of the most environmentally important materials. It plays a critical role in weather, where it seeds many forms of precipitation, affects climate, and impacts geology and life in polar regions. The surfaces of ice have unique chemical and physical properties, including the formation of a quasi-liquid layer due to surface melting, and proton disordering inside the ice crystal. The hydrogen bonding network of water molecules governs ice nucleation processes and provides a unique platform for catalytic reactions, particularly those involving stratospheric ozone depletion. Recent methodological advances in theoretical and experimental chemistry provide the ability to characterize the structure and dynamics of ice and have increased global interest in investigating the properties of ice across several disciplines. This symposium will focus on experimental and theoretical progress in our understanding of the structure and dynamics of the ice surfaces, biological and abiotic ice nucleation, and the chemistry of hydrates. This symposium will provide a platform for updates on the progress of each of these areas, thereby stimulating collaborations and advancing our understanding of the chemistry of ice.

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Physical Chemistry of Ionic Liquids

Ionic liquids continue to be the focus of intense research activity in many areas of chemistry, including nanoscience, biomaterials, and separation technologies. Energy-related applications include batteries, supercapacitors, dye-sensitized solar cells, separations of gases (CO_2, H_2, etc.), rare earth elements and spent nuclear fuel, desulfurization, biofuels, fuel cells, and catalysis. Ionic liquids encompass a very broad range of possible components, affording a diverse combination of tunable properties for fundamental science investigations and practical applications that promote sustainability by enabling advanced technologies. This symposium will convene a community of experts in the physical chemistry and chemical physics of ionic liquids to discuss the continued expansion of ionic liquids research activity into many areas of science and technology. Since the mid-2000s, physical chemistry has played a pivotal role in understanding how ionic liquids function by elucidating their structure, dynamics, phase and solvent properties, etc. These advances have greatly benefitted the applications-oriented side of the ionic liquid community, and changed the way we understand higher-temperature molten salts, which are currently being intensely investigated for their use as heat transfer fluids in solar thermal power installations, molten salt nuclear reactors, and blankets for fusion reactors.

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Physical Chemistry of Molecular Electronics

The concept of using molecules as electronic components has been historically motivated by the miniaturization of integrated circuits in line with Moore's Law. It is now recognized that molecular devices can demonstrate properties unique from those in conventional electronics, resulting from quantum interference effects, changes in molecular redox state, and/or the immediate nanoscale environment. With robust and reproducible measurement techniques now established and great gains made in reconciling experimental and theoretical results, attention has turned to the discovery of useful wires, switches, diodes, and resistors – and how best to utilize them. This symposium will create a fertile ground for gathering a global cohort of researchers together to discuss the latest discoveries, exchange ideas, and develop collaborations and networks across four distinct, yet strongly interconnected areas: single-molecule measurements, large-area measurements, theory, and synthesis. Appropriate topics include, but are not limited to, single-molecule conductance experiments; large-area molecular electronic device characterization; first principles calculations of molecular charge transport; integrating molecules into functional circuits; and synthetic routes to molecular electronic components.

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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: 2 October 2023 **http://abstracts.acs.org**

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