CALL FOR PAPERS

PHYS Physical Chemistry
ACS Technical Division

ACS DIVISION OF PHYSICAL CHEMISTRY
FALL 2025 NATIONAL MEETING
AUGUST 17-21, 2025
WASHINGTON, DC

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 January 7 and closes on March 31, 2025**. 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.

Prospects of Quantum Computing for Quantum Chemistry

The rapid advancements in quantum computing have led to increased research on quantum algorithms and applications, with quantum chemistry emerging as a key area for potential breakthroughs. Quantum computing offers the ability to efficiently simulate complex chemical reactions and materials, promising to transform the design of new materials, catalysts, and drugs. This symposium brings together the quantum computing research community to share findings and tackle challenges in the field. It emphasizes the interdisciplinary nature of this research, featuring talks from experts in quantum and classical computing and fundamental studies addressing challenges in quantum chemistry. The program includes educational content on quantum computing software and hardware and a panel discussion on the future of quantum computing in chemistry. The symposium aims to advance the field through collaboration among researchers, educators, and industry professionals in quantum computing for chemistry and materials science.

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Spectroscopic Imaging, Multi-dimensional Spectroscopy, and Nanospectroscopy

This symposium brings together experimentalists and theoreticians advancing modern spectroscopy and spectroscopic imaging to explore structures, dynamics, and reactivity in gases, clusters, liquids, solids, and their interfaces. Topics include advanced spectroscopy and microscopy techniques such as non-conventional chemical imaging, tip-enhanced Raman, nano-infrared spectroscopy, time-resolved and multi-dimensional infrared and electronic spectroscopy, and their theoretical foundations. Applications span chemistry, energy, biology, environment, and functional materials, alongside theoretical and computational methods linking spectroscopic data to their chemical and physical origins. Advanced spectroscopy and imaging offer unparalleled spatial and temporal resolution, transforming our understanding of molecular and material composition, organization, interactions, and dynamics at extreme scales. This symposium fosters knowledge exchange, networking, and interdisciplinary collaborations within the larger community, driving progress across diverse fields.

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Automation & Artificial Intelligence for 2D Materials Discovery

This symposium highlights experimental advancements in the autonomous and semi-autonomous identification, manipulation, and measurement of two-dimensional (2D), van der Waals materials. Topics include recent progress in hardware, software, and experimental techniques for characterizing 2D materials and creating heterostructures and devices. Special focus will be placed on breakthroughs in artificial intelligence, such as computer vision and machine learning, and their use in automating the collection, labeling, and analysis of large experimental datasets. The symposium facilitates cross-disciplinary discussions among researchers exploring diverse materials and device applications, with insights from fields like biological sciences and computer science. Sessions will cover the physical tools and techniques employed in autonomous 2D materials experiments, alongside control software and data processing strategies, fostering collaboration and innovation in this rapidly evolving area.

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Rare Event Sampling in Material Science Problems: From Fundamental Understanding to Technological Applications

This symposium focuses on advancements in rare event sampling techniques applied to complex material science and soft matter phenomena. These methods are crucial for simulating low-probability but high-impact events such as phase transitions, chemical reactions, and conformational changes, which are key to understanding diverse materials and soft matter systems. The symposium will cover state-of-the-art methodologies and applications, including enhanced sampling techniques like metadynamics, umbrella sampling, and transition path sampling; multiscale modeling; and Markov state models. Discussions will also address theoretical frameworks and algorithmic innovations for efficiently exploring high-dimensional phase spaces and capturing rare events with greater accuracy. The symposium fosters interdisciplinary collaboration among experimentalists and theorists/simulators, with topics spanning solvation dynamics, chemical reactions in solution, biomolecular interactions, environmentally relevant processes, and polymer physics. It provides a platform for sharing insights and advancing rare event sampling methods across condensed matter systems.

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Embedding methods for ground and excited states

Embedding is a powerful approach for studying complex systems with electronic structure theory, reducing computational cost as system size increases. Early methods combined semi-empirical quantum mechanics for enzyme active sites with molecular mechanics or continuum models, and recent advancements in QM/QM, QM/MM, fragmentation, and PCM methods have enhanced their sophistication. Applications in electronic excitations and nonadiabatic dynamics, essential for photochemistry and photobiology, have driven innovations in coupling the QM region with its environment. Subsystem interactions, once treated classically, are increasingly captured explicitly with embedding operators. Modern software development, GPU hardware, machine learning, and enhanced sampling techniques enable simulations of larger QM regions and longer timescales. Embedding methods now span materials science, biomolecules, condensed-phase dynamics, spectroscopy, and catalysis. This symposium features embedding methods for diverse systems, with talks from experts advancing and applying these methods across chemistry, biochemistry, and materials science.

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Chenchen Song, UC Davis ccsong@ucdavis.edu
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Michele Pavanello, Rutgers-Newark m.pavanello@rutgers.edu

Molecular level understanding of structure and dynamics at electrochemical interfaces

This symposium addresses experimental and theoretical advancements in understanding structure, dynamics, and elementary processes at electrochemical interfaces. Efficient energy conversion requires functional electrodes that catalyze complex multi-electron reactions, actively binding reactants, stabilizing intermediates, and enabling inner-sphere electron transfer. However, a molecular-level understanding of these processes remains limited, hindering progress in developing more efficient energy technologies. Tackling this challenge demands integrated approaches combining operando probes and atomistic simulations to build multiscale models of interfacial phenomena. The symposium highlights recent progress in experimental techniques, theoretical models, and simulations for molecular-level insights into interfacial structure, dynamics, and reactions. Topics include interfacial fields, solvation, vibrational energy relaxation, charge and energy transfer, proton-coupled electron transfer, and electric field effects. Advances in in situ and operando spectroscopic and imaging methods will be featured, fostering collaboration between experimentalists and theoreticians to drive innovation in electrochemical energy conversion.

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Bridging Theory and Experiment with AI

This symposium highlights advancements in integrating artificial intelligence (AI) with theoretical and experimental chemistry to solve complex problems, accelerate discovery, and enhance understanding of chemical processes. Key themes include AI-driven theoretical chemistry, showcasing how AI models are applied to quantum mechanics, molecular simulations, and molecular dynamics for new theoretical insights. In experimental chemistry, discussions will focus on AI's role in automating experiments, analyzing data, predicting outcomes, and optimizing conditions. The symposium will also explore data-driven chemistry, emphasizing machine learning at the interface of theory and experiment, and highlight collaborations between theorists, experimentalists, and AI researchers that have led to breakthroughs. Ethical considerations, data management, and reproducibility challenges in AI-driven research will also be addressed. This symposium aims to inspire innovation and foster collaborations, providing a platform for knowledge exchange and advancing the intersection of AI and chemical sciences.

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Sergei Treatiak, Sergei Treatiak, LANL serg@lanl.gov

Nanoscale tools to understand the physical biology of a cell

Advancements in biochemical and molecular research have illuminated cellular functions, yet nanoscale tools to manipulate and study cells have been limited. The emergence of nucleic acid nanotechnology probes now enables the exploration of biophysical behaviors in the extracellular space, cell membrane, and intracellular components. Synthetic DNA nanostructures and devices, with their self-assembling properties, biocompatibility, and versatility, have significantly advanced the understanding of cellular forces, behaviors, and transport. Nanoscale tools such as “calipers,” membrane engineering structures, and phase-separated coacervates made from synthetic DNA/RNA can dynamically interact with biological systems. This symposium will showcase cutting-edge biophysical tools utilizing synthetic nucleic acid nanotechnology to programmatically interface with cellular environments, offering novel insights into cellular processes.

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Alexander Marras, University of Texas at Austin amarras@utexas.edu
Carlos Castro, The Ohio State University castro.39@osu.edu

Closing the Gap between Light and Matter: Advances in Plasmonics and Beyond

This symposium focuses on advancing chemical conversion, sensing, and material science through the exploration of light-matter interactions. Bringing together researchers from academia and industry, it bridges fundamental experiments, theoretical insights, and practical applications to drive scientific discovery and technological innovation. Topics include driving chemical reactions via hybridized light-matter interactions, understanding interactions at single and sub-particle levels, leveraging strong light-matter interactions for advanced sensors, and developing new materials for future photonic applications. While emphasizing contributions in plasmonics, the symposium welcomes topics from related fields, fostering inclusive discussions on shared principles. By engaging researchers from various areas of physical chemistry, the symposium aims to facilitate knowledge exchange, interdisciplinary connections, and networking opportunities within the larger scientific community, catalyzing progress in the study of light-matter interactions.

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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: 31 March 2025 **http://abstracts.acs.org**

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