CALL FOR PAPERS

ACS DIVISION OF PHYSICAL CHEMISTRY

NATIONAL ACS MEETING

San Antonio, TX ☺ 21-25 March 2021

The Division of Physical Chemistry is hosting the following oral symposia, consisting of both invited and contributed papers, as well as a general poster session. **The abstract submission deadline has yet to be announced (usually late October), so keep checking this PDF for updates**.
For those interested in an oral presentation, please submit abstracts to the appropriate symposium. 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.

SYNERGY BETWEEN QUANTUM COMPUTING AND HIGH-PERFORMANCE COMPUTING IN QUANTUM CHEMISTRY AND MATERIALS SCIENCE

Quantum simulation is the emulation by a controlled quantum system of another quantum system of interest. Simulation of quantum systems is commonly performed on high-performance computers, with efficient codes that exploit modern computer architectures. The scale of manageable systems at the quantum level of theory has grown from a few atoms to few thousands of atoms in the past century, yet this scale is still far from the natural scale of problems in biomedicine, drug design, and materials science/engineering. Quantum simulation could potentially bypass the size limitations, opening the exploration of quantum effects in life sciences and industrial technologies. Quantum simulation also bears the promise to overcome current methodological approximations that limit our understanding and control of materials and chemical dynamics. This symposium brings together quantum scientists, materials scientists, and quantum chemists to discuss the synergies between high-performance computing and quantum computing in these fields. It will feature tutorials on quantum hardware and the software used to interact with these systems by experts in the field.

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GRAPH THEORY UNDERPINNING NEW DOMAINS OF PHYSICAL CHEMISTRY

Graph theory has experienced recent growth in various applications in Chemistry, yet the broader community remains unaware of its impact in a range of new fields, including the domain of reaction networks, sub-ensemble analysis and interfacial chemistry, materials design and synthesis and the study of energy landscapes. While major emphases lie within the area of Machine Learning as a mainstay of Data Science, graph theory methods and topological data analysis in general, are emerging as cutting-edge tools for pattern recognition and the ability to leverage graph patterns to make close connections to underlying chemical phenomena. This symposium offers a wide view of recent developments in the application of graph or network theory algorithms to learn about complex energy landscapes, hierarchical and emergent phenomena and as a basis for new theoretical methodologies that leverage pattern recognition to increase scalability. The symposium integrates multiple disciplines to provide a platform for physical chemists learning from advancements made from the fields of catalysis, biophysics, mathematics and vice versa.

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THE CHEMISTRY OF MOLECULAR ELECTRONICS

The concept of using molecules as electronic components has received significant attention over the past 3 decades, initially motivated by the decreasing size of semiconductor-based circuit elements in line with Moore's Law. It is now recognized that molecular devices can demonstrate properties unique from those observed 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 multi-disciplinary symposium will bring together research in molecular electronics from synthesis, single-molecule measurements, large area measurements and theory. Topics include: Synthetic routes to molecular electronic components; Single-molecule conductance experiments; Large-area molecular electronic device characterization; First principles calculations of molecular charge transport; and Integrating molecules into functional circuits.

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DYNAMICS OF CHEMICAL REACTIONS FROM GAS PHASE TO INTERFACES: A SYMPOSIUM IN HONOR OF PROFESSOR WILLIAM L. HASE

Professor William Hase, formerly the Welch Chair and Horn Professor at Texas Tech University, has made significant contributions in Physical Chemistry, including quasi-classical trajectory approaches to uni- and bi-molecular scattering, RRKM rate theory for unimolecular reactions, non-statistic dynamics in organic reactions, energy transfer, and surface scattering. He has been a true champion in prompting multidisciplinary research combining theory, computation and experiments. The impact of his scientific work and his service to physical chemistry have been broad, deep and long lasting. In memory of his untimely passing in March, 2020, this symposium is organized to bring together Professor Hase's peers, young independent researchers, and students in these fields to discuss the current research and future directions. The speakers include current leaders in both experiment and theory around the world and the topics cover uni- and bi-molecular reaction dynamics and energy exchange, surface chemistry and dynamics, and biological molecules and interactions with engineered materials.

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ASTROCHEMICAL COMPLEXITY IN PLANETARY SYSTEMS

Through the use of increasingly sensitive remote and in-situ observational techniques, our knowledge of interstellar and planetary environments has dramatically increased over the last few decades. The ongoing development of new spacecraft missions, multi-wavelength, ground-based observatories and pioneering laboratory techniques promises significant advances in our knowledge of chemical complexity in the Universe in the coming decades. Understanding and interpreting these new data requires dedicated computational efforts. Analytical techniques are becoming increasingly sensitive, with several methods offering: i) sub-femtomolar detection levels, ii) spectroscopy at nanometer spatial resolution, iii) emerging 3D tomography techniques approaching atomic resolution, and iv) novel correlated multi-technique or multi-dimensional technique approaches. Since astronomical samples are in very limited supply, it is essential that the developers of these techniques collaborate/coordinate with planetary scientists to maximize the utility of this work. Accordingly, this symposium aims to bring together astrochemists and planetary scientists with expertise in observations, sample analysis, laboratory experiments, planetary missions, and development of novel analytical techniques, and theoretical modeling. The aim is to identify frontier research areas and foster new, interdisciplinary collaborations to promote a deeper understanding of how and where chemical complexity arises on planetary surfaces.

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2D MATERIALS FOR ENERGY, SENSING, AND QUANTUM INFORMATION SCIENCE

2D materials with atomic scale thickness have emerged as a new frontier in physics, chemistry and materials science. While graphene has attracted attention in the previous decade, the current decade has witnessed a meteoric rise in the diversity of compositions, properties and applications of 2D materials beyond graphene. In most cases, the properties and applications of non-graphene 2D materials go far beyond those of graphene. Given the recent scale of developments and activity in this field, this symposium is dedicated to promoting communication among researchers working on 2D materials beyond graphene including physical chemistry, materials science, surface science, inorganic chemistry, computational studies and device engineering. Topics will include the synthesis and assembly of 2D materials and related heterostructures, 2D materials for light harvesting, catalysis and energy storage, 2D material-based hybrids, computational studies with 2D materials and 2D materials for quantum information science.

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STRUCTURE AND DYNAMICS OF AMYLOIDS AND PRECURSORS BY NMR

The process by which proteins form amyloid fibrils plays a crucial role in many diseases, but is also increasingly understood to have functional roles in many organisms. The structural basis for the formation of amyloid, and the structure of the precursors and intermediate states are thus of extreme interest. One of the best methods to understand structures throughout this process is NMR spectroscopy, which will be the focus of this symposium. In addition to the more well-known disease associated amyloids, we will also host a session on functional amyloids, these systems aggregate like all amyloids but in a well-controlled manner. The process of aggregation begins with smaller oligomers. Many proteins undergo oligomerization but only some go on to form amyloids. The dynamic process by which proteins form oligomers which then turn into larger aggregates is well suited for study by NMR.

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EMERGING TECHNIQUES TO PROBE CONDENSED PHASE DYNAMICS ACROSS TIME AND SPACE

Biological and materials systems are replete with complex phenomena that arise from a variety of dynamical processes. These dynamics are challenging to characterize and understand as they depend on a range of molecular parameters, occur on multiple timescales, and are spatially heterogeneous. In recent years, innovations in the methodology of ultrafast spectroscopy have enabled resolution of these dynamics through the introduction of spatial resolution, increases in spectral bandwidth, and improvements in optical design. These advances have led to new insights into relationships between structure and function in materials like inorganic nanostructures, organic semiconductors, and photosynthetic proteins. This symposium will focus on developments in ultrafast science to describe excited state dynamics, and the applications of these new approaches.

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EXPERIMENTAL AND COMPUTATIONAL APPROACHES IN UNRAVELING MECHANISMS OF AMYLOID FORMATION

Amyloid fibrils, insoluble materials associated with diseases are chemically diverse and yet adopt similar β-sheet rich fibril structures at the ultrastructural level. A number of factors have been identified to play essential roles in early stages of the protein aggregation process such as variations in sequence and posttranslational modifications. Environmental factors like metal ions and phospholipid membranes are also recognized to be important in catalyzing oligomerization and modulating aggregation. This symposium will bring together research scientists from several domains of experimental and theoretical physical chemistry to discuss and explore open questions in the field such as fibril polymorphism and cross-seeding. The synergy between computation and experiment in this symposium will facilitate collaborative discussions towards new method development and identification of promising approaches for the future.

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SINGLET FISSION MATERIALS AND MECHANISMS FOR SOLAR ENERGY CAPTURE AND CONVERSION

Singlet fission is a multi-exciton generation mechanism that offers the potential to overcome thermodynamic limits in traditional solar energy capture and conversion systems. However, achieving this potential in practical applications requires predictive design rules about how molecular structure, energetics, and coupling influence the properties of multi-exciton and correlated triplet pair intermediates, their spin decoherence, and yield for triplet separation, transport and harvesting. This symposium will bring together a synergistic group of people working at the forefront of mechanistic experimental and computational studies, synthesis of new materials, and hypothesis-driven applications of singlet fission. The role that spin-exchange, decoherence and energetics have on the rate and yield of correlated triplet pair separation and extraction of triplet excitons will be a particular focus. Recent work demonstrating the potential to utilize coherent pathways to influence the rate and yield particularly of endergonic singlet fission systems will be explored.

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MOLECULAR CRYSTAL POLYMORPHISM: HOW, WHEN, AND WHY MOLECULES PACK IN THE SOLID STATE

Molecular crystal polymorphism contributes to phenomena ranging from pharmaceutical solubility to the taste of chocolate. Screening pharmaceutical polymorphs, designing organic semiconductors, investigating energetic materials, or solving challenging crystal structures involves many obstacles where computational modeling could help. This symposium will focus on the theoretical challenges associated with modeling molecular crystals, where the simultaneous need to model the molecular interactions with high accuracy and to sample configurations and/or crystal structures thoroughly requires creative new approaches. Key themes will include crystal structure prediction, structure refinement and energy ranking, and the statistical mechanics of polymorphism, nucleation, and growth. Perspectives from experimental researchers will be included who can highlight the current state of the art in these fields and identify outstanding challenges.

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PHYSICAL CHEMISTRY POSTER SESSION

Contributions from all areas of physical chemistry are highly encouraged for the poster session. Up to six 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: XX OCTOBER 2020 http://abstracts.acs.org

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FOR INFORMATION ABOUT THE PHYSICAL CHEMISTRY DIVISION, VISIT OUR WEBSITE: **http://phys-acs.org/**