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 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 tens of thousands of atoms in the past century, yet this scale is still far from the natural scale of biochemistry and drug discovery, 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 chemical behavior - to the extent that the modern theoretical chemist, 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.

Rosa De Felice, University of Southern California, rdefelice@usc.edu
Truls Haugland, University of Oslo, truls.haugland@ntnu.no
Bert De Jong, Lawrence Berkeley National Laboratory, wade@philips.gov
Gables, Cameron, University of Texas at Austin, cameron.gables@utexas.edu
James Whitfield, Darmouth University, james.d.whitfield@darmouth.edu

GRAPH THEORY UNPINNING 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, ensemble analysis of molecular systems, and modern molecular modeling. A major emphasis lies 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 identify structural features relevant to the physical behavior of matter. The 25th International Symposium on Molecular Sciences focuses on the use of increasingly sensitive remote and in situ observational techniques, our knowledge of chemical complexity arising on planetary surfaces.

The abstract submission deadline has yet to be announced (usually late October), so keep checking this PDF for updates.

This symposium aims to bring together research, lab, and in situ observational techniques, our knowledge of chemical complexity arising on planetary surfaces.

For those interested in an oral presentation, please submit a 250-word abstract by the deadline listed below. Selections will be made by February 28, 2021. notified. The contributions not selected for oral presentations will be assigned to the poster session.

The Division of Chemistry is hosting the following oral symposia, combining 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.

Synergy between Quantum Computing and High-Performance Computing in Quantum Chemistry and Materials Science

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

2D materials with atomically thin thickness have emerged as a new frontier in physics, chemistry and materials science due to the unique electronic, optical, mechanical and magnetic properties beyond those of graphene. In recent years, this class of materials has shown great potentials for applications 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, theoretical calculations, material design, device innovation, 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 applications of 2D materials in quantum information science.

Mirece Cotlet, Brookhaven National Laboratory, cotlet@bnl.gov
Deep Jariwala, University of Pennsylvania, jariwalad@seas.upenn.edu
Donald DeMarzio, Northrop Grumman, donald.de_marzio@ngc.com

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. The only methods to understand structures throughout this process is NMR spectroscopy, which will be the focus of this symposium. In addition to the well-known amyloid diseases such as Alzheimer's disease, 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 dynamics leading to protein aggregation are key to understanding the potential for forming amyloids for study by NMR.

Jean Baum, Rutgers University, baum@chem.rutgers.edu
Andrew J. Nieuwkoop, Rutgers University, nieuwkoop@chemistry.rutgers.edu

EMERGING TECHNIQUES TO PROVE 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 parameters such as temperature, pressure, and time scales. Therefore, multi-disciplinary approaches are needed. In recent years, improvements in the methodology of ultrafast spectroscopy have enabled resolution of these dynamics through the introduction of new photolysis methods and the development of novel laser technology. The symposium aims to bring together researchers involved in these fields to explore and discuss the development of new methodologies to study dynamical processes in biological and materials systems.

Gabriela Schlau-Cohen, Massachusetts Institute of Technology, gschlau@mit.edu
Cathy Wong, University of Oregon, cathywong@oregon.edu

EXPERIMENTAL AND COMPUTATIONAL APPROACHES IN UNRIVELING MECHANISMS OF 2D MATERIALS FOR LIGHT FORMATION

2D materials with atomic scale thickness have emerged as a new frontier in physics, chemistry and materials science due to the unique electronic, optical, mechanical and magnetic properties beyond those of graphene. In recent years, this class of materials has shown great potentials for applications 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, theoretical calculations, material design, device innovation, 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 applications of 2D materials in quantum information science.

Mirece Cotlet, Brookhaven National Laboratory, cotlet@bnl.gov
Deep Jariwala, University of Pennsylvania, jariwalad@seas.upenn.edu
Donald DeMarzio, Northrop Grumman, donald.de_marzio@ngc.com

SINGLET FISON MATERIALS AND MECHANISMS FOR SOLAR ENERGY CAPTURE AND STORAGE

Singlet fission is a multi-excitation-generation mechanism that offers the potential to overcome thermodynamic limits in traditional solar energy capture and conversion systems. However, achieving this potential in practical solar cells is hindered by several material, device, and methodological challenges. For example, the properties of multi-exciton and correlated triplet pair intermediates, their spin-dissociation, and yield for triplet separation, transport and harvesting. This symposium will bring together synergic groups of people working at the forefront of 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.

Jean Baum, Rutgers University, baum@chem.rutgers.edu
Andrew J. Nieuwkoop, Rutgers University, nieuwkoop@chemistry.rutgers.edu