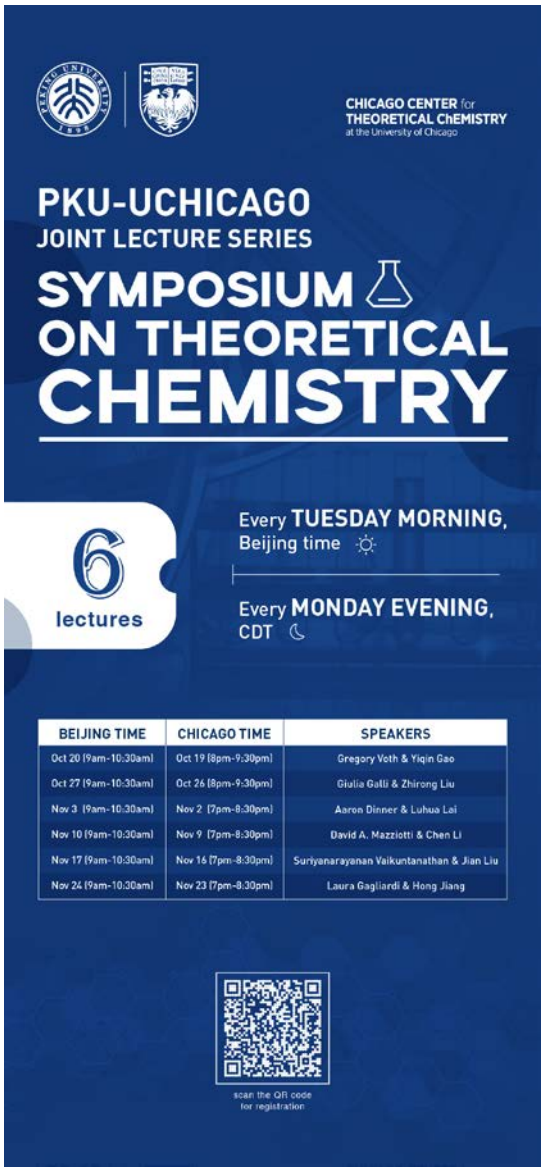
PKU-UChicago Joint Series: Symposium on Theoretical Chemistry

Lecture 2:
Quantum Simulations of Heterogeneous Materials on Classical and Near-term Quantum Computers
&
Ensemble-based Thermodynamics of the Fuzzy Binding between Intrinsically Disordered Proteins and Small Molecule Ligands: Principle and Application



Speakers:
Giulia Galli, University of Chicago
Zhirong LIU, Peking University
Moderator:
Chen LI, Peking University

Time:
October 26, 8:00 pm (CDT)
October 27, 9:00 am (Beijing time)

Series Description: The Symposium on Theoretical Chemistry will explore the concepts and underlining principles of chemistry through discourse between faculty from the Chicago Center for Theoretical Chemistry at the University of Chicago and Peking University. The series will create an open dialogue about computational theories and methods, and their applications. The symposium will advance conversations in the field of modern theoretical chemistry and include discussions on biophysics, quantum dynamics, electronic structure theory and non-equilibrium statistical mechanics, among others.

Speakers from this joint lecture series are co-chaired by faculty members from Peking University and the University of Chicago. The lectures will be held every Tuesday morning Beijing time and every Monday evening Chicago time. Please scan the QR code or click the link below for registration.

Registration Link:
https://uchicago.zoom.us/webinar/register/WN_eGh5QNeSQKGL-KKFWcFOsA

Giulia Galli is the Liew Family professor of Electronic Structure and Simulations in the Pritzker School of Molecular Engineering and Professor of Chemistry at the University of Chicago. She also holds a Senior Scientist position at Argonne National Laboratory (ANL) and she is the director of the Midwest Integrated Center for Computational Materials (MICCoM). Prior to joining UChicago and ANL, she was Professor of Chemistry and Physics at UC Davis (2005-2013) and the head of the Quantum Simulations group at the Lawrence Livermore National Laboratory (1998-2005). She holds a Ph.D. in Physics from the International School of Advanced Studies (SISSA) in Trieste, Italy. She is a Fellow of the American Physical Society, the American Association for the Advancement of Science and the American Academy of Arts of Sciences, as well as a member of the National Academy of Sciences. She is a recipient of numerous awards, including the Lawrence Livermore National Laboratory Science and Technology Award, the US Department of Energy Award of Excellence, the Materials Research Society Theory Award, the APS David Adler Lectureship in Materials Physics, the Feynman Nanotechnology Prize in Theory, the medal of the Schola Physica Romana and the Tomassoni-Chisesi award by the Sapienza University of Rome. Her research activity is focused on the development and use of theoretical and computational methods to understand and predict the properties and behavior of materials (solids, liquids, and nanostructures) from first principles.

Title:

Quantum Simulations of Heterogeneous Materials on Classical and Near-term Quantum Computers

Abstract:

In this talk Prof Galli will present strategies to predict and design materials for next generation technologies by combining theories based on quantum mechanics, and algorithms and codes running on high performance classical computers, and, in some cases, on near-term quantum computers. She will present examples of calculations addressing two outstanding challenges: designing sustainable materials to efficiently capture solar energy, and inventing materials to build radically novel sensors and computers, to move in earnest into the quantum information age.

Zhirong LIU received his Ph.D. in condensed matter physics at Tsinghua University in 2001. He acted as a postdoctoral guest scientist in Max Planck Institute for Metals Research in 2001-2002 to study nanostructure in alloy thin films. Then he worked on the electronic-structure theory under electric field in the Center for Advanced Study at Tsinghua University as a temporary researcher for a short time before he switched to the biophysics field. In 2003-2007, he worked on protein folding, DNA conformational statistics and related energetics in University of Toronto as a postdoctoral scholar in Prof. Hue Sun Chan's group. In July, 2007, he joined College of Chemistry and Molecular Engineering, Peking University as an associate professor, and later was promoted to full professor in 2015. His current research focuses on the molecular modeling and calculation of chemical systems: (1) molecular recognition of intrinsically disordered proteins; (2) electronic structure and electron-phonon-photon interactions in two-dimensional materials; (3) applications of machine learning in chemistry. Dr. Liu has published over 120 peer-reviewed journal articles.

Title:

Ensemble-based Thermodynamics of the Fuzzy Binding between Intrinsically Disordered Proteins and Small Molecule Ligands: Principle and Application

Abstract:

The "lock-and-key" model is the basis of molecular recognition concerning biological macromolecules and played an essential role in the long-term success of drug development. However, intrinsically disordered proteins (IDPs), which exist in an ensemble of rapidly changing conformations and exhibit almost unlimited structural heterogeneity, have brought challenge to the conventional paradigm. How is a key able to match locks with different shapes? More scientifically, how to properly access the binding affinity between a small molecule ligand and a conformational ensemble of proteins? In our work, we presented an ensemble-based thermodynamic framework to analyze the fuzzy ligand-IDPs interactions. It is shown that the apparent affinity acts in a way similar to the Jarzynski's equality in nonequilibrium statistics. The oncoprotein c-Myc is adopted as an example to demonstrate the related properties, e.g., the distribution of conformation-ligand interaction free energy, the entropic contribution from the ensemble, the conformation shift under ligand binding, and how to control the error under a limited number of sampled conformations. In addition, we proposed a reinforcement learning algorithm for virtual screening upon IDPs, which greatly reduces the docking number while achieving both high screening accuracy and low performance loss.