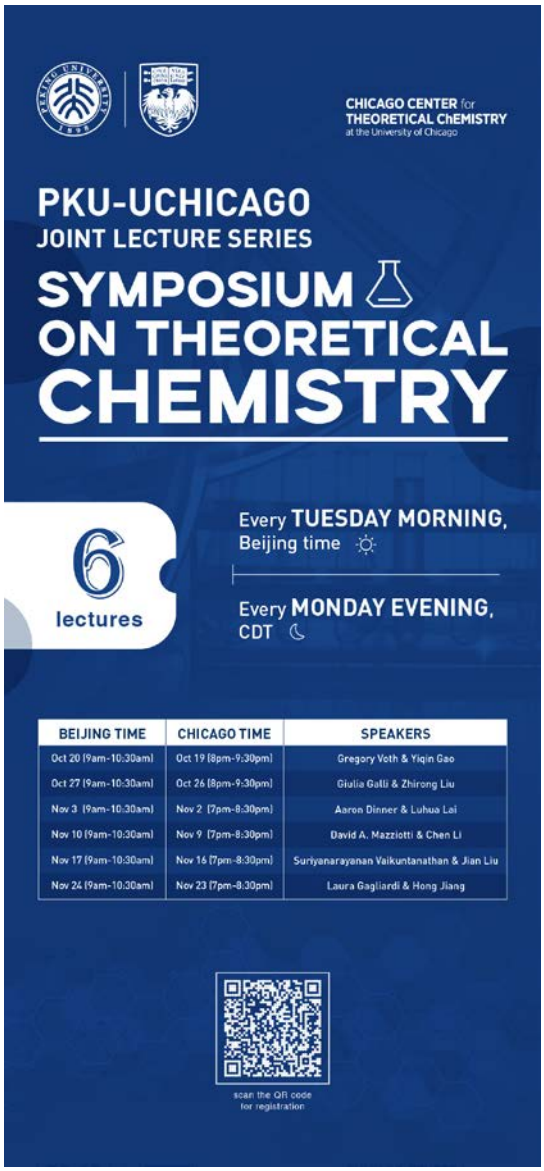
PKU-UChicago Joint Series: Symposium on Theoretical Chemistry

Lecture 1: Frontiers of Biomolecular Theory & Simulation



Speakers:
Gregory Voth, University of Chicago
Yiqin Gao, Peking University

Moderator:
Chen LI, Peking University

Time:
October 19, 8:00 pm (CDT)
October 20, 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.

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

Gregory A. Voth is the Haig P. Papazian Distinguished Service Professor of Chemistry at The University of Chicago. He is also a Professor of the James Franck Institute and the Institute for Biophysical Dynamics. He received a Ph.D. in Theoretical Chemistry from the California Institute of Technology in 1987 and was an IBM Postdoctoral Fellow at the University of California, Berkeley from 1987-89. He is the author or co-author of more 535 peer-reviewed scientific articles that have been cited more than 42,000 times with a current h-index of 103. Voth is a Fellow of the American Chemical Society, American Physical Society, The Biophysical Society, the Royal Society of Chemistry, and the American Association for the Advancement of Science. He has received a number of awards and other forms of recognition for his work, including most recently the Joel Henry Hildebrand National American Chemical Society Award in the Theoretical and Experimental Chemistry of Liquids, the Royal Society of Chemistry S.F. Boys-A. Rahman Award for Outstanding Innovative Research in Computational Chemistry, and the American Chemical Society Division of Physical Chemistry Award in Theoretical Chemistry. He has mentored more than 200 postdoctoral fellows and graduate students. Professor Voth is a leader in the development and application of theoretical and computational methods to study problems involving the structure and dynamics of condensed phase systems, including proteins, membranes, liquids, and materials. He has pioneered the theory and simulation of complex multiscale problems, including early use of machine learning for multiscale molecular problems ~20 years ago before it was called by that name.

Title: Overcoming the Multiscale Simulation Challenge for Biomolecular Systems

Abstract:
Advances in theoretical and computational methodology will be presented that are designed to simulate complex (biomolecular and other soft matter) systems across multiple length and time scales. The approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of these concepts are methods for deriving coarse-grained (CG) models from molecular structures and their underlying atomic-scale interactions. This particular aspect of the work has strong connections to the procedure of renormalization in physics, but in the context of CG models it is developed and implemented for more heterogeneous systems. An important new component of our work has also been the concept of the "ultra-coarse-grained" (UCG) model and its associated computational

implementation. In the UCG approach, the CG sites or “beads” can have internal states, much like quantum mechanical states. These internal states help to self-consistently quantify a more complicated set of possible interactions within and between the CG sites, while still maintaining a high degree of coarse-graining in the modeling. The presence of the UCG site internal states greatly expands the possible range of systems amenable to accurate CG modeling, i.e., quite heterogeneous systems, including complex self-assembly processes involving large multi-protein complexes. Applications to experimentally important targets such as cytoskeleton actin filaments and virus particles (virions) will be given.

Yi Qin Gao is a Professor at College of Chemistry and Molecular Engineering and an investigator at the Biomedical Pioneering Innovation Center，Peking University. He received his B.S. degree from Sichuan University, his M.S degree from Institute of Chemistry, Chinese Academy of Sciences, and his Ph.D from California Institute of Technology. He was a postdoctoral fellow at Caltech and Harvard University from 2001 to 2004. He was an assistant professor at the chemistry department of Texas A&M University from 2005 to 2009 and moved to Peking University in 2010. He is currently a member of editorial board of J. Chem. Phys., J. Phys. Chem., Chem. Phys. Lett., ACS Central Sci., and Mat. Of Chem.

Title: Analysis of the DNA sequence dependence in the high order chromatin structure formation

Abstract: The high-order chromatin structure plays an important role in gene regulation. The mechanism, especially the sequence dependence for the formation of varied chromatin structures in different cell states remain to be elucidated. In this talk, we try to touch on three questions: (1) What is the sequence dependence and chemical structure basis in the formation of high order chromatin structure, ranging from open chromatin to compartments? (2) How does the chromatin structure reflect the biological function of different cellular states and tissue-specificity? (3) How does this sequence-dependent chromatin structure formation manifest in different species? Based on the sequence properties, we divided the genome into two sequentially, epigenetically, and transcriptionally distinct regions. These two megabase-sized domains were found to spatially segregate, and to different extents in different cell types. They show enhanced segregation from each other in development, differentiation, and senescence, meanwhile the

multi-scale forest-prairie spatial intermingling is cell-type specific and increases in differentiation, helping to define cell identity. We propose that the domain segregation of the 1D mosaic sequence in the 3-D space serves as a potential driving force, and together with cell type specific epigenetic marks and transcription factors, shapes the chromatin structure in different cell types. Specifically, based on the analysis of latest published Hi-C data of post-implantation stages, we present a consistent view of the chromatin structural change and the corresponding sequence dependence. We will also discuss the possible chromatin structure changes in carcinogenesis.