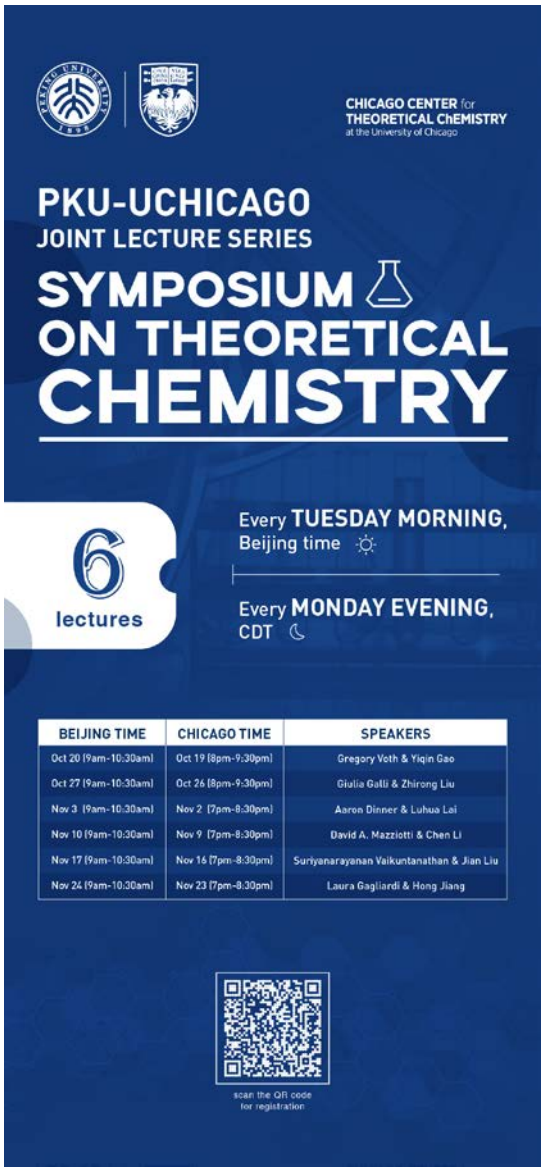
PKU-UChicago Joint Series: Symposium on Theoretical Chemistry

Lecture 3: Complex Reaction Mechanisms and Drug Design



Speakers:
Aaron Dinner, University of Chicago
Luhua Lai, Peking University

Moderator:
Chen LI, Peking University

Time:
November 2, 7:00 pm (CDT)
November 3, 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

Aaron Dinner is a Professor of Chemistry and Deputy Dean of the Physical Sciences Division at the University of Chicago. He also holds appointments in the Institute for Biophysical Dynamics and the James Franck Institute, the latter of which he was Director previously. His group's most well-known contributions are to machine learning methods for interpreting complex biomolecular simulations, sampling methods for systems far from equilibrium, models of hematopoietic cell fate choice, and quantitative studies of cytoskeletal dynamics. Much of his current work is collaborative, and many of his students and postdoctoral scholars are jointly mentored by experimentalists and/or applied mathematicians. Professor Dinner's honors include a Searle Scholarship, NSF CAREER Award, Sloan Fellowship, and APS Fellowship. Prior to joining the faculty at the University of Chicago, he obtained his undergraduate and graduate degrees at Harvard University; subsequently, he pursued postdoctoral studies at the University of Oxford and University of California, Berkeley.

Title: Systematic methods for learning complex mechanisms from molecular dynamics simulations

Abstract: Computers and algorithms are now sufficiently powerful that many complex molecular processes can be simulated at atomic resolution. Yet it remains challenging to describe dynamics when processes are stochastic, proceed by multiple pathways, and involve collective motions. In this talk, I will present recent work that we have done to advance methods for efficiently estimating chemical kinetic statistics and systematically learning complex reaction mechanisms from molecular dynamics data. Applications to understanding protein folding and ligand binding will be presented.

Luhua Lai is a professor at the College of Chemistry and Molecular Engineering, Peking University and an investigator at the Center for Quantitative Biology and Peking-Tsinghua Center for Life Sciences, Peking University. She received a B.S in 1984 and a Ph.D. in 1989 from Peking University. She was a Berkeley Scholar in the University of California at Berkeley in 1999-2000. She is on editorial board of BMC Bioinform., J. Med. Chem., J. Mol. Recognit. and Quant. Biol. Her group is focused on developing computational methods and apply them in drug design and functional protein design.

Title: From structural to systems-based drug design

Abstract: Structural based drug design has been widely used in drug discovery for lead identification and optimization. However, drugs encounter many biological molecules in human body and systematic modeling of drug actions is necessary. In this talk, Prof. Lai will present their work on metabolic network modeling, intervention strategy analysis, and novel drug design methods development for protein activator design and multiple target drug design.