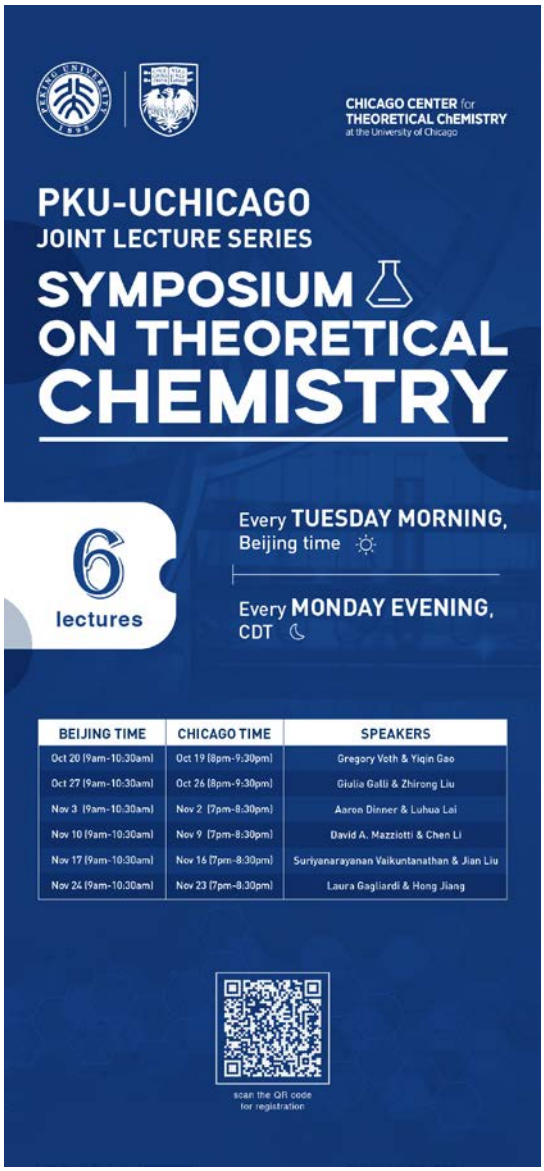
PKU-UChicago Joint Series: Symposium on Theoretical Chemistry

Lecture 5: Non-equilibrium Thermodynamic and Quantum Dynamics

Speakers:
Suriyanarayanan Vaikuntanathan, University of Chicago
Jian LIU, Peking University

Time:
November 16, 7:00 pm (CDT)
November 17, 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

Suriyanarayanan Vaikuntanathan is the principal investigator of the Vaikuntanathan Group at the University of Chicago. The group pursues projects related to solvation thermodynamics and the statistical mechanics of self-assembly in a number of systems ranging from lipid membranes to nanocyrstals in ionic melts. His current research is focused on the development and use of tools of equilibrium and non-equilibrium statistical mechanics to understand the behavior of complex systems in physical chemistry, soft condensed matter physics, and biophysics.

Vaikuntanathan received his degree in Biotechnology from the Indian Institute of Technology-Madras in 2006 and a Ph.D. in Chemical Physics from the University of Maryland in 2011. He was a Postdoctoral Fellow in Prof. Phillip Geissler's group at the University of California, Berkeley and joined the University of Chicago in 2014. He received the Camille Dreyfus Teacher-Scholar Award in 2020, an NSF Career Award in 2018, and an Alfred P. Sloan Fellowship in 2017, among others.

Title: Design principles for controlling organization and self-assembly far from equilibrium

Abstract: Understanding the microscopic chemical and physical principles that control organization and self-assembly in non- equilibrium conditions remains an important problem in statistical mechanics. In this talk, I will describe recent work from my group that elucidates how non-equilibrium forces can be used to achieve novel self-assembly, functionality and organization in a variety of chemical and biological systems. I will focus in particular on two new non-equilibrium thermodynamic frameworks developed in the group and show how these can be used to achieve control over morphologies, material properties and self-assembly in wide range of microscopic non-equilibrium systems. Together, our results lay the framework for a general set of thermodynamic principles to control transport, assembly and organization in a broad class of non-equilibrium systems

Jian Liu obtained B.S. (2000) from the University of Science & Technology of China and then Ph.D. (2005) from the University of Illinois at Urbana-Champaign. He worked as a postdoctoral fellow at the University of California, Berkeley and then Stanford University, before he was appointed Associate Professor at the College of Chemistry and Molecular Engineering, Peking University. He was a recipient of the Pople Medal of the Asia-Pacific Association of Theoretical and Computational Chemists (2019). Professor Liu's research deals with quantum and semiclassical theories of chemical dynamics and thermodynamics for real molecular systems.

Title: Rational design for trajectory-based methods for quantum statistics and dynamics

Abstract: Unraveling nuclear quantum effects in dynamic, spectroscopic and thermodynamic properties of complex molecular systems has long been challenging in modern physical chemistry. In this context, I will describe some recent progress in my research group:
(1) Path integral molecular dynamics (PIMD) for quantum statistics. We employ the Kolmogorov operator to develop a unified framework that covers both stochastic and deterministic thermostatting algorithms. In this framework, most conventional PIMD algorithms can be unified in the "side"/"end" schemes. More importantly, the "middle" scheme for PIMD proposed by us significantly improves the sampling efficiency as well as accuracy for general molecular systems.
(2) Path integral Liouville dynamics (PILD) for quantum dynamics. Derived from the elaborate combination of the imaginary time path integral and phase space formulation of quantum mechanics, PILD is a practical quantum dynamics method satisfying the two critical fundamental criteria: conservation of the quantum Boltzmann distribution for the thermal equilibrium system and being exact for any thermal correlation functions (even of nonlinear operators, i.e., nonlinear functions of position or momentum operators) in the classical and harmonic limits.