Getting Something for Nothing: Classical and Machine-Learning Methods for Quantum Simulation

SPEAKER: Thomas F. Miller III, California Institute of Technology
TIME: 2:00pm-3:00pm, Wednesday, August 28, 2019
VENUE: Room 264, Geography Building, Zhongbei Campus, ECNU
HOST: Xiang Sun, NYU Shanghai

ABSTRACT OF THE TALK
A focus of our research is to develop simulation methods that reveal the mechanistic details of quantum mechanical reactions that are central to biological, molecular, and heterogeneous catalysis. The nature of this effort is three-fold: we combine quantum statistical mechanics and semiclassical dynamics methods to expand the scope and reliability of condensed-phase quantum dynamics simulation; we develop quantum embedding and machine learning methods that improve the description of molecular interactions and electronic properties; and we apply these methods to understand complex chemical systems.

The talk will focus on recent developments and applications of Feynman path integral methods for the description of non-adiabatic chemical dynamics, including long-ranged electron transfer in proteins and gas-surface collisions. Additionally, we will describe a machine-learning approach to predicting the electronic structure results on the basis of simple molecular orbitals properties, yielding striking accuracy and transferability across chemical systems at low computational cost.

BIOGRAPHY
Thomas Miller’s research focuses on the development of theoretical and computational methods to study chemical processes that are related to catalysis, battery technologies, and membrane protein biosynthesis. After completing his undergraduate studies at Texas A&M University, he attended graduate school in the UK on a British Marshall Scholarship and received his Ph.D. from Oxford University in 2005. Miller then returned to the US for a postdoctoral fellowship at UC Berkeley. He joined the faculty of the California Institute of Technology in 2008 and was promoted to full professor in 2013. While at Caltech, he has received awards that include the Sloan Research Fellowship, NSF CAREER Award, Associated Students of Caltech Teaching Award, Dreyfus Teacher-Scholar Award, and the ACS Early-Career Award in Theoretical Chemistry.