Classical and Machine-Learning Methods for Quantum Simulation

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A focus of my 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 work from the foundation of quantum statistical mechanics and semiclassical dynamics to develop methods that significantly 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 [1] and applications [2] of Feynman path integral methods for the description of non-adiabatic chemical dynamics, including proton-coupled electron-transfer and long-ranged electron transfer in protein systems. Additionally, we will describe a machine-learning approach [3] 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.

