Classical and Machine-Learning Methods for Quantum Simulation

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A focus of our research is to the develop simulation methods that reveal the mechanistic details of quantum mechanical reactions that are central to biological, molecular, and heterogenous 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 [1] and applications of Feynman path integral methods for the description of non-adiabatic chemical dynamics, including long-ranged electron transfer in proteins [2] and atom-surface collisions [3]. Additionally, we will describe a machine-learning approach [4,5] 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.

References

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