Chemistry Colloquium

Wednesday, October 27, 12:00 pm

140 Hutchison Hall, Lander Auditorium

*Livestream option available for those unable to attend in person

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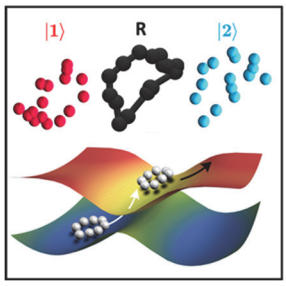
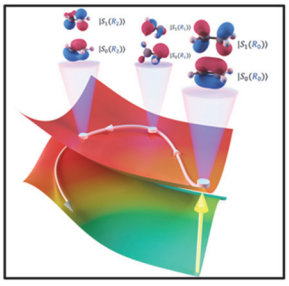
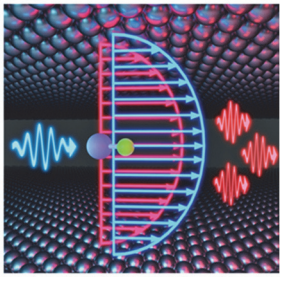
"*Quantum Dynamics of Light-Matter Interactions*"

Abstract: Strong couplings between molecules and quantized photon fields have the potential to facilitate new chemical reactivities. Theoretical investigations of such quantum transitions among these electron-photon hybrid states are beyond the scope of photochemistry or quantum optics and remain a challenge in theoretical chemistry. In this talk, I'll present several new theoretical approaches that address these challenges. First, I'll discuss our recently derived non-adiabatic ring polymer molecular dynamics approach, which provides a unified theoretical framework to accurately describe electronic non-adiabatic dynamics and nuclear quantum effects. Second, I'll introduce the quasi-diabatic propagation scheme that provides a seamless interface between adiabatic electronic structure calculations and diabatic quantum dynamics approaches, facilitating the development of new on-the-fly simulation techniques. Finally, I'll present our recent investigations on new chemical reactivities enabled by cavity quantum electrodynamics and demonstrate detailed mechanisms of how quantized light-matter interactions can change the outcomes of chemical reactions.







*** Livestream option available via Zoom:** https://rochester.zoom.us/j/95034670629

Website: https://events.rochester.edu/event/chemistry_colloquium_huo