PHYSICAL SEMINAR

Manifestation of Spin-Orbit and Electron-Nuclear Couplings in Computational Molecular Spectroscopy

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UNIVERSITY OF WASHINGTON
Host: Prof. Yang Yang

The computational modeling of molecular spectroscopies requires an accurate treatment of spin-orbit and electron-nuclear couplings to fully understand the physical underpinnings of the spectroscopic signatures. In this talk, I will briefly review recent developments in relativistic electronic structure theory and electron-nuclear quantum dynamics from the Li research group, followed by computational studies of several advanced molecular spectroscopies and challenging chemical processes. L- and M-edge X-ray absorption, where large spin-orbit coupling splits the core p/d orbitals into several sublevels, can now be computed with relativistic electronic structure methods developed in the Li research group. These new methods can provide extremely important insights into chemical processes involving transition metal, rare earth, and heavy elements. In order to study the effect of quantum proton, we have developed the nuclear-electronic orbital Ehrenfest (NEO-Ehrenfest) dynamics, in collaboration with the Hammes-Schiffer group. NEO-Ehrenfest provides an elegant framework for treating electrons and selected nuclei, typically protons, quantum mechanically in nonequilibrium dynamical processes, such as the excited state intramolecular proton transfer process. Our simulations reveal that nuclear quantum effects influence the predictions of proton transfer reaction rates and kinetic isotope effects due to the intrinsic delocalized nature of the quantum nuclear wave function.

DATE: TUESDAY, FEBRUARY 8th, 2022
TIME: 11:00 am in the Learning Center, Room 1435

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