
J. Clarence Karcher

Lecture

◆DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY ◆THE UNIVERSITY OF OKLAHOMA
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We Are Pleased to Announce a Seminar
Presented By

Xiaosong Li
University of Washington

Friday, January 20, 2023
4:15 pm
NWC 1313

Manifestation of Spin-Couplings in Computational Molecular Spectroscopy

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.

Refreshments will be served.
(abstract on back)

Dr. Li received his Ph.D. in Chemistry from the Wayne State University in 2003 and following a post-doctoral training at the Yale University, he joined the University of Washington in the fall of 2005. He is a dual appointee and Lab Fellow at Pacific Northwest National Laboratory and serves as the Executive Director of the NSF MRSEC Molecular Engineering Materials Center. He is the Larry Dalton Endowed Chair in Chemistry and the Associate Vice Provost for Research Cyberinfrastructure. Internationally recognized for his work in time-dependent quantum theory and relativistic electronic structure methods, Dr. Li has a passion for collaborative research and his project portfolio is prolific. His research products are clear evidence of his passion for sponsored research; he has amassed 250 peer-reviewed publications and developed several computational software packages with >12,000 publication citations and >60,000 software citations. He has received awards that include the Sloan Research Fellowship, National Science Foundation CAREER Award, Fellow of the American Physics Society, elected member of the Washington State Academy of Sciences, and the University of Washington Distinguished Teaching Award.