Special Guest Lectures

A Multi-Stage Ab-initio Wavepacket Dynamics Formalism for Electronic Structure and Dynamics in Open Systems

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Frey Computing Services Building 307
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Abstract:
In this talk, we discuss the Multi-Stage Ab-initio Wavepacket Dynamics (MS-AIWD) Formalism for the study of delocalized electronic systems as well as electron transport through donor-bridge-acceptor systems such as those found in molecular-wire/electrode networks. The full donor-bridge-acceptor system is treated through a rigorous partitioning scheme that utilizes judiciously placed offsetting absorbing and emitting boundary conditions. These facilitate a computationally efficient and potentially accurate treatment of the long-range coupling interactions between the bridge and donor/acceptor systems, and the associated open-system boundary conditions. The quantum dynamics of the electronic flux through the bridge-donor/acceptor interface is constructed using an accurate and efficient representation of the discretized quantum-mechanical free-propagator. A model for an electrode-molecular wire-electrode system is used to test the accuracy of the scheme proposed. Transmission probability is obtained directly from the probability density of the electronic flux in the acceptor region.

Speaker's Bio:
Alexander B. Pacheco is currently a postdoctoral fellow in the Department of Chemistry at Indiana University. He received his Ph.D in Chemistry from University of Florida; his M.Sc. in Physical Chemistry from University of Pune; and his B.Sc. in Chemistry from University of Mumbai. Pacheco's current research interests are: 1) Investigation of electronic transport properties in molecular wire systems, 2) developed a multistage Ab-Initio wavepacket dynamics scheme for donor-bridge-acceptor systems to study electron dynamics in open systems such as Molecular Electronic Devices; 3) calculations were carried out by modifying existing code for Wavepacket Dynamics on a model potential to obtain transmission coefficient and spectra of electronic flux flowing through the bridge system as a function of initial kinetic energy; 4) theoretical investigation of Intermolecular Vibrational Energy Redistribution for reactions of atmospherically important molecules with radicals.

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