Novel Approaches Beyond Born-Oppenheimer Separation to Capture Nuclear-Electronic Couplings

Seminar

Thursday, March 13, 2025

10:45 – 11:45 a.m.

Beaupre Center, Room 105

The Born-Oppenheimer (BO) approximation, which separates the motions of electrons and nuclei, is foundational to our understanding of electronic structures, molecular spectroscopy, and reaction dynamics. However, there are critical cases where this separation breaks down, necessitating approaches that go beyond the BO framework.

In this research talk, I will present two novel methods that address non-BO nuclear-electronic couplings from distinct perspectives. The first, the nuclear-electronic orbital (NEO) method, captures quantum effects such as zero-point energy and proton tunneling by treating key protons and electrons on an equivalent footing. The second approach, the electronic phase-space Hamiltonian, incorporates electronic couplings with nuclear momentum, recovering missing electronic momentum and vibrational circular dichroism (VCD) spectra absent in the BO approximation. Additionally, the latter captures momentum transfer between nuclei and electronic spin, potentially important for chiral-induced spin selectivity (CISS). These two methods are applicable to a wide range of chemical and biological systems, including systems with spin, where nuclear-electronic coupling is crucial but often not well understood.

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Spring 2025 Seminar Series

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