UCMERCED | CHEMISTRY & BIOCHEMISTRY

DATE 10/18/2024 | TIME 01:30pm | LOCATION COB1 267

CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES:

Phase Space Approaches to Electronic Structure: A New Paradigm For Chiral Induced Spin Selectivity

Abstract:

The Born-Oppenheimer approximation is the cornerstone of chemistry, the idea that electronic structure and molecular orbitals are defined relative to a stationary set of coordinates for the nuclei. This premise is based on the important differences in mass between electrons and nuclei, and the all important fact that nuclei move much slower than electrons and appear effectively frozen on the time scale of electronic fluctuations. Nevertheless, it is known that the Born-Oppenheimer approximation breaks down quite often, quite famously in the context of photochemistry and/or electron transfer. Slightly less well known is the fact that a classical BO theory does not conserve momentum (linear or angular) even when there is no obvious breakdown. In this talk, I will discuss this failure of the BO approximation, offer up phase space approximations as an improvement to restore conservation, and then suggest a new paradigm for understanding how nuclear entanglement with electronic degrees of freedom may well lead to chiral induced spin selectivity (an exciting phenomenon discovered in recent years).

Joseph Subotnik

Professor of Chemistry

Princeton University

About the Speaker:

Joe Subotnik is a Professor of Chemistry at Princeton University. He graduated from Harvard (BA, physics) in 2000 and from Berkeley (PhD, biophysics) in 2007. He was an NSF postdoctoral fellow in Israel from 2007-2010, and was previously a Professor of Chemistry at the University of Pennsylvania (2010-2024). His research focuses on developing tools to describe energy conversion, the manner by which electrons, photons and nuclei exchange energy and angular momentum, especially in the condensed phase, merging fundamental chemical physics with practical computational methods. He has made fundamental contributions to the semiclassical surface hopping algorithm, the theory of electronic friction at metal surfaces, and the theory of vibrational circular dichroism.

For more info, contact: Christine Isborn cisborn@ucmerced.edu