DEPARTMENTS OF CHEMISTRY
Seminar Series

FRIDAY, September 18, 2026 - 12:00 Noon
MC H313

Chemical Bonds and Molecular Properties

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Essentially all spectroscopic, optical, electric, and magnetic properties of molecules can be calculated as derivatives of the energy or a time-averaged quasi-energy. The derivatives are taken with respect to electric and magnetic field amplitudes, electronic and nuclear magnetic moments, nuclear positions, and so on. Furthermore, the calculated properties can be decomposed into contributions from individual molecular orbitals, which provides relationships between observed properties and the chemical bonding & molecular structure. I will discuss the analysis of these relationships by using examples taken from past and on-going research of optical activity, NMR parameters, NMR chemical shifts of paramagnetic molecules, and X-ray absorption spectra of lanthanides and actinides. Time permitting, I will also show results from our projects on radicals with 'non-aufbau' configurations and discuss the accuracy of of so-called density-corrected DFT for molecular properties.