

HIGHLANDS IN CHEMISTRY SEMINAR SERIES



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“Strong correlations and symmetry-breaking in molecules”

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2:30PM

ZOOM

FACULTY HOST:
GRADUATE STUDENTS

We think about the electronic structure of molecules in terms of molecular orbital (MO) theories, such as mean-field Hartree-Fock (HF) theory, or most commonly, Kohn-Sham density functional theory (DFT). Both HF and DFT use a single determinant wavefunction of MOs: the MOs are 1-electron energy levels that are either occupied or empty, and changes in the occupied orbitals control chemical reactivity. The mean-field picture, with small refinements via DFT works very well for perhaps 95% of molecular applications of quantum chemistry.

What about the small percentage of molecules for which the mean-field orbital picture breaks down? Such systems are said to have strongly correlated electrons, since HF neglects electron correlations. In strongly correlated systems, orbitals are fractionally occupied, and the wavefunction is intrinsically multi-determinant, and the formal compute complexity is exponential with the number of entangled electrons (on a classical computer, at any rate).

This talk will first be concerned with understanding some basic aspects of strongly correlated molecules by way of introduction. This provides an introduction to some research on a method to diagnose the presence of strong correlations without needing to use a multi-determinant wavefunction. In the process, we will consider carefully the connections between symmetry-breaking and strong correlations, that form part of the famous “symmetry dilemma” of quantum chemistry. With these considerations in hand, we will then focus on some interesting molecules including fullerene, C_{60} , that are claimed to be strongly correlated, and see to what extent those claims can be supported or contradicted using the new diagnostic.