Title: Developments in Quantum Chemistry for Molecular Excited States: Spectroscopy and Dynamics using DFT/MRCI

Abstract:
I will discuss developments by our group in multi-reference electronic structure methods for molecular excited states based on the combined Density Functional Theory / Multi-reference Configuration Interaction approach. These techniques are designed to fill a niche in the description of molecular excited states: possessing the computational efficiency of density functional based methods, but combined with the generality and quantitative accuracy of multi-reference CI. Furthermore, the "black-box" nature of these methodologies lend themselves to widespread use in a variety of application areas. I will here present a number of such applications, including the simulation of: UV absorption and ionization spectra involving multiple electronic states, X-ray absorption and photo-electron spectra, and time-resolved spectroscopic experiments involving the ultrafast evolution of wave packets involving strong coupling between vibrational and electronic degrees of freedom.