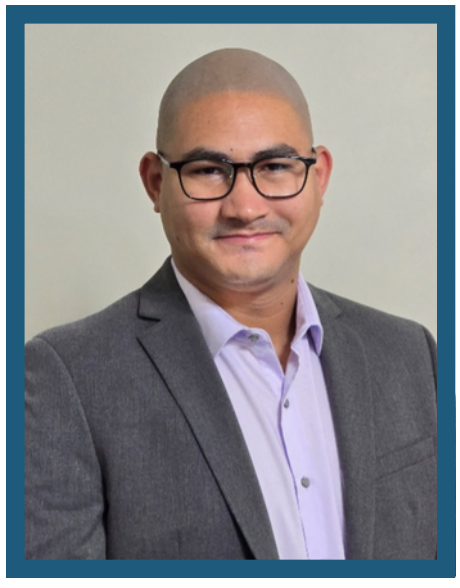
HIGHLANDS IN CHEMISTRY SEMINAR SERIES



Professor Daniel Nascimento

University of Memphis

"Exploring quasi-relativistic density functional theory approaches in the simulation of resonant inelastic x-ray scattering maps"

October 3, 2025

2:30 PM ET

Hahn Hall North 140

Experimental advancements are pushing the boundaries of core-level spectroscopy. Modern light sources can now produce unprecedented ultrafast x-ray laser beams that can be used to probe chemical processes occurring on the femtosecond timescale with extraordinary resolution. These technologies allow us to gather valuable time-resolved information about the electronic structure of atoms and molecules. However, the theoretical tools commonly used to interpret and analyze the wealth of data produced by light source facilities are heavily reliant on model Hamiltonians, thus lacking predictive ability. While high-level, predictive quantum chemistry techniques, such as coupled-cluster theory would be highly desirable in this context, these techniques remain too computationally expensive for routine use on systems larger than a few dozen atoms. An attractive alternative is to employ density functional theory (DFT) and its variants, as they have been shown to perform reasonably well for a large number of systems at an affordable computational cost.

In this talk, I will present our ongoing efforts to develop and apply DFT-based methods for simulating near-edge x-ray fine structure (NEXAFS) and resonant inelastic x-ray scattering (RIXS) in transition metal complexes. I will focus on how quasi-relativistic approximations based on the zeroth-order regular approximation can be constructed to efficiently incorporate scalar-relativistic and spin-orbit effects, and how these strategies can be extended to simulate multi-dimensional core-level spectra.