UNIVERSITY OF RHODE ISLAND
Department of Chemistry
SEMINAR

Room 105 Beaupre Center
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Dr. Daniel Nascimento

PNNL

"Exploring time-domain coupled-cluster methods for simulating the linear electronic spectra of molecules"

HOST

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Exploring time-domain coupled-cluster methods for simulating the linear electronic spectra of molecules

Coupled-cluster theory is highly regarded as the “gold standard” of quantum chemistry due to its robustness and accuracy in predicting molecular properties. Nonetheless, it often leads to computational methods that are too expensive (in terms of computing time and memory requirements) to be applicable to molecules containing more than a few non-hydrogen atoms. This limitation is particularly problematic in the simulation of spectroscopic properties, where more than one state needs to be considered in the computation.

In this talk, I will present some of our most recent contributions to the development of efficient computational approaches for simulating electronic spectra of molecules within the linear response regime. These approaches are based on a time-domain formulation of coupled-cluster theory, which when compared to conventional frequency-domain formulations, are shown to significantly reduce both the memory consumption and computing time without compromising accuracy. These savings are especially valuable when simulating high-energy spectra, as in extreme ultra-violet and near-edge X-ray absorption fine structure (NEXAFS) spectroscopies or describing spectral features that involve many excited electronic states.