Department of Physics
UCF
PHYSICS COLLOQUIUM

Speaker: Dr. Kenneth Lopata, Louisiana State University

An Attochemistry Picture of Electron Dynamics

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Abstract: At the attosecond time scale, short intense laser pulses can induce electronic dynamics in molecules that occur faster than nuclear motion. This motion forms the initial steps of important processes such as photochemistry and light harvesting, but many questions remain concerning the properties of a molecule that give rise to nontrivial attosecond dynamics, and how it can be observed experimentally. In this talk, I will present time-dependent density functional therory (TDDFT) simulations of two exemplar classes of this: (i) charge migration, where valence electron holes move in a particle-like manner following strong-field ionization of a molecule, and (ii) core-hole induced dynamics, where sudden soft X-ray ionization results in coherent valence electron motion faster than the Auger-Meitner decay time. In these contexts, dynamics in both organic molecules (e.g., functionalized benzene) and inorganic (transition metal) complexes will be discussed, each of which offer unique advantages and properties for experiments. Some technical and validation details will be discussed, but the main emphasis of this talk will be to draw conclusions about how the structure of a molecule regulates the dynamics in a chemically intuitive way. Indeed, our results suggest that a density-based picture and simple attochemistry principles are fruitful for predicting and interpreting CM in complex systems.

BIO: Dr. Lopata is computational chemist specializing in attosecond electron dynamics. He earned his Ph.D. in Chemistry from the Univeristy of California, Los Angeles, where he created new methods for understanding coupled molecule/plasmon interactions. Following that, he did a postdoc at Pacific Northwest National Laboratory, where he developed computational approaches and codes for simulations spectra and electron dynamics in molecules. Currently, he is Professor at Louisiana State University in the Department of Chemistry, where his work focuses on using simulations to understand how electrons move in molecules, and how they respond to high intensity and/or energy laser light. He has published over 50 peer-reviewed papers, and is a recipient of the Department of Energy Early Career Award.