Kenneth Lopata - 2017 DOE Early Career Awardee

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Assistant Professor Ken Lopata has received an Early Career Award from the US Department of Energy (DOE). This program, now in its eighth year, supports the development of individual research programs of outstanding scientists, at universities and national laboratories, early in their careers and stimulates research careers in the disciplines supported by the DOE Office of Science. The grant is for $750,000 for a period of 5 years, starting September 2017, from the Basic Energy Sciences Division..

Dr Lopata is an expert at first-principles simulations of the motion of electrons during and immediately following the interaction of matter with high energy and/or high intensity light. Since Lopata began his independent career at LSU in the Department of Chemistry and the Center for Computation and Technology (CCT) in Fall 2013, Dr Lopata has developed time-dependent density functional theory (TDDFT) methods for a range of processes including: UV-Visible and X-ray spectroscopy, strong-field ionization, plasmon/molecule dynamics, and attosecond charge migration. These simulations are crucial for elucidating excited state mechanisms in molecules and solid-state materials, interpreting ultrafast time-resolved experiments, and for motivating new directions as the drive towards faster experimental time resolutions continues.

First Principles Tools for Nonadiabatic Attosecond Dynamics in Materials

Controlling materials at the level of electrons, and characterizing and controlling matter far-from-equilibrium, are two ongoing grand challenges in solid-state science. These have the potential to revolutionize fields ranging from energy storage to conversion of light into electrical and chemical energy. In particular, the mechanisms of ultrafast light-induced changes in solids are poorly understood at an atomic level. These dynamics occur at the attosecond (billionth of a billionth of a second) time scale and involve a complex interplay of electron motion coupled to the movement of the atoms in a crystal lattice.

The objective of this research is to develop computer simulation tools for predicting the ultrafast response of materials subjected to intense pulses of light. This is crucial for understanding the underlying mechanisms and for interpreting and motivating attosecond experiments. There is a lack of first-principles approaches for this type of dynamics, especially for photochemistry-like processes near dopants and defects. This project will develop density functional theory-based methods for attosecond electron/nuclear dynamics in semiconductors and insulators under the influence of high intensity and/or high energy (X-ray) laser pulses. These will be validated against experiments and enable computation of optical breakdown, electron/lattice couplings, excited state lifetimes, and the origins of non-thermal damage.

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