Special Guest Lectures

First-principles Ultrafast Chemical Dynamics

Kenneth Lopata, Pacific Northwest National Laboratory

Johnston Hall 338
March 22, 2013 - 09:00 am

Abstract:

Light-matter interactions, excited states, and femtosecond-scale chemical dynamics underpin a wide range of important physical processes such as light harvesting, photochemistry, and charge/energy dynamics in materials. Especially interesting, but poorly understood from a theory standpoint are multi-photon and strong-field processes, where the external fields can have intensities on the order of the internal molecular fields (e.g., near plasmons). Here, first principles quantum chemistry virtual "experiments" offer the unique ability to directly visualize electronic and nuclear motion at their natural length and time scales during the evolution of an excited state. In this talk I will discuss real-time time-dependent density functional theory (RT-TDDFT) and highlight how it can be used to shed light on excitations in aromatic molecules, doped titania, and charge injection dynamics in dye sensitized solar cells. Additionally, high performance computing aspects will be discussed, including integration in the massively parallel Free/Open Source computational chemistry package NWChem.

Speaker's Bio:

Kenneth Lopata was selected to receive the first William Wiley Distinguished Postdoctoral Fellowship at the Department of Energy's EMSL. He worked with scientists in the NWChem development team within EMSL's High Performance Software Development group. The Fellowship is awarded to candidates who display superb ability in scientific research and show promise to become outstanding leaders in their research field.

He received his PhD in Physical Chemistry from UCLA in June 2010 under the supervision of Professor Daniel Neuhauser.

Center for Computation & Technology
2003 Digital Media Center • Telephone: +1 225/578-5890 • Fax: +1 225/578-8957