Time-dependent density functional theory studies of electron dynamics in plasmonic systems

Christine M. Aikens, Ph.D.
Department of Chemistry, Kansas State University, Manhattan, KS, 66502, USA

Plasmonic systems such as silver nanoparticles are of interest for applications such as plasmon-enhanced photocatalysis and as waveguides. In order to improve the efficiency of these processes, we must understand how energy flows throughout the system and how energy transfers between two nanoparticles or between a nanoparticle and adsorbate. In this work, we present our studies that employ real-time time-dependent density functional theory (RT-TDDFT), often combined with the nonadiabatic Ehrenfest method, to examine plasmon decay and electronic energy transfer processes. We investigate electron-nuclear dynamics in systems such as silver nanowires and acenes, which display collective effects analogous to those in nanoparticle systems. We assess the non-linear excitations in tetrahedral silver nanoparticle systems. In addition, we analyze how plasmonic excitation in nanoparticle systems leads to bond activation and photocatalysis.