Theory and plasmons: going beyond conventional classical electrodynamics

George C. Schatz
Northwestern University

This talk will describe our recent efforts to improve on classical electromagnetic theory in the description of metal nanostructure (plasmonic) optical properties, with emphasis on surface enhanced optical properties that are relevant to Raman and solar energy. A top-down approach involves the use of nonlocal dielectric response in classical electrodynamics. We have recently developed a method for embedding the hydrodynamic Drude model (a nonlocal dielectric model) into the finite-difference time domain method. This allows us to study the optical properties of both very small particles and of small gaps between big particles at a higher level than in past work, including for single-electron excitations as well as plasmon excitations in the same theory. The bottom-up theory that we use is real time (RT) time dependent density functional theory (TDDFT). Here I will describe a series of projects that we have done that enables us to describe the optical properties of metal clusters with up to 1000 atoms, which makes it possible to observe the convergence of electronic structure results to the bulk electrodynamic limit. The direct coupling of electronic structure theory with electrodynamics (multiscale calculations) will also be examined.