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Abstract for an Invited Paper for the MAR08 Meeting of the American Physical Society

Quantum Mechanics and Electrodynamics Studies of the Optical Properties of Metal Clusters/Nanoparticles GEORGE SCHATZ, Northwestern University

This talk will describe the use of electrodynamics and quantum mechanics methods to describe the optical properties of silver and gold nanoparticles and other nanostructures. This work has been done in collaboration with several experimental colleagues, including Chad Mirkin, Rick Van Duyne and Teri Odom. Our recent work has focused on the optical properties of metal nanoparticles that are coated with molecules that are detected either through their influence plasmon resonance excitation, or via surface enhanced Raman spectroscopy (SERS). Electrodynamics calculations using either the DDA or FDTD methods provide a quantitative tool for characterizing far field properties, and at a more primitive level estimates of SERS intensities. Quantum mechanics, as developed using time dependent density functional theory, is restricted to small metal clusters, but the same methods of far field spectroscopy and SERS can still be studied.