Optical Properties of Semiconducting and Metallic Nanoparticle Structures by TDDFT

EMILY TOWNSEND, GARNETT BRYANT, National Institute of Standards and Technology — Superstructures of semiconducting and metallic nanoparticles display substantially novel properties compared to homogeneous materials or single nanoparticles due to the coupling of elementary excitations between different nanoparticles, i.e. the confined plasmons in the metallic nanoparticles and excitons in semiconductor quantum dots. We use time-dependent density functional theory (TDDFT) to examine the optical response of such structures. This method allows a quantitative, fully quantum mechanical treatment of the electronic response of both the semiconducting and metallic components.