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Plasmonic Response of Metallic Nanoparticles by Time Dependent Density Functional Theory EMILY TOWNSEND, GARNETT BRYANT, Joint Quantum Institute, National Institute of Standards and Technology and Univ of Maryland — Plasmons in metallic nanoparticles (MNPs) hold the potential to carry quantum information. Exploiting this will require a quantum understanding of plasmons in hybrid structures of multiple MNPs and emitters/absorbers. We use real-time, real-space time dependent density functional theory (TDDFT) to examine resonances in the optical response of single and paired MNPs. We consider the character of different resonances (some occur in the core, others near the surface of the MNP) and examine the multiple excitations that constitute these resonances. In both the core and surface resonances we see both plasmon-like sloshing of electrons around the Fermi surface and single-particle-like excitation of electrons from below the Fermi surface to above it. We examine the resonances of a pair of MNPs as a function of their separation distance to see how plasmonic and single-particle excitations mix in these particles. Widely separated pairs behave similarly to individual MNPs, but at closer distances pairs behave like a single, more complicated system.

Emily Townsend
Joint Quantum Institute, National Institute of Standards
and Technology and Univ of Maryland

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