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Multiscale Electrodynamics/Time-Dependent Density Functional Theory Modeling of Coupled Plasmon/Molecule Excitations[1] KENNETH LOPATA, HOLDEN SMITH, Louisiana State University, Department of Chemistry — The coupled dynamics of molecular chromophores and plasmons at surface of metal nanostructures are important for a range of processes such as molecular sensing, light harvesting, and near-field photochemistry. Modeling these dynamics from first principles, however, is challenging, as the large system sizes precludes a purely quantum mechanical treatment. In this talk I will present an approach based on propagating the plasmonic currents and fields using electrodynamics (finite-difference time-domain) with each chromophore described using an isolated quantum sub-region embedded in the overall classical background. This approach can be readily parallelized over these quantum regions, which enables large multiscale simulations of tens or hundreds of dyes, each of which is described individually by real-time time-dependent density functional theory. Application to gold nanoparticles coated with malachite green and rhodamine 6G monolayers shows good agreement with experimentally measured coupling spectra, including the polariton peaks, as well as the plasmon and molecular depletions.

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Kenneth Lopata
Louisiana State Univ - Baton Rouge

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