Molecular nanoplasmonics

Michael Galperin

University of California San Diego, Department of Chemistry & Biochemistry, 9500 Gilman Dr., La Jolla, CA 92093-0340, USA

Advances in optical techniques, in particular nearfield optical microscopy, combined with molecular fabrication techniques, make optical spectroscopy methods an important observation and diagnostic tool in molecular electronics. The molecular optical response in close proximity to plasmonic materials is greatly enhanced by surface plasmon-polariton modes leading to the discovery of the single-molecule spectroscopy. A natural combination of nanoplasmonics and molecular response to the generated field started to appear as molecular nanoplasmonics. In particular, it is a natural ingredient in any study of molecular junctions interaction with light. The small size of molecules implies necessity of quantum treatment ofmolecular junctions response to external driving, while macroscopic size of contacts (nanoparticles) requires to rely on the tools of classical electrodynamics in simulation of plasmon excitations in the leads.

Within simple models we present simulations of time-dependent transport and optical response of molecular junctions driven by external laser fields. First we persent results of simulations employing combination of nonequilibrium Green functions for description of the molecule and finite difference time-domain approach for numerical integration of Maxwell equations on a spatial grid [1]. We demonstrate effects of pulse chirping ond energy relaxation on charge pumping properties in molecular junctions [2], and study local field formation due to both surface plasmon-polariton excitations in the contacts and the molecular response [3]. In the second part of the talk we discuss a possible route for quantum description of the coupling between plasmons and molecular excitons in junctions. In particular, we employ a pseudoparticle nonequilibrium Green function formalism to study the sensitivity of the molecule-plasmon Fano resonance to junction bias and intramolecular interactions, and compare our predictions to previous studies [4].

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