Localized surface plasmons and their interaction with molecules: first-principle and hybrid modeling approaches

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First principle methods such as time-dependent density functional theory are gaining ground in the investigation of localized surface plasmons (e.g., supported by metallic nanoparticles) and their effects on the optical properties of nearby molecules (e.g., surface-enhanced spectroscopies). On one hand, they can be used to address basic questions such as the microscopic nature of the plasmonic excitations themselves (what distinguish a plasmon from single-particle or excitonic excitations?). On the other hand, hybrid models can be devised for molecules close to metal nanoparticles, where the molecule is treaded by a first principle method and the nanoparticle as a continuous dielectric.

Here I shall present our work related to first-principle and hybrid approaches to localized surface plasmons and their interaction with molecules. In particular, I will discuss our proposals to characterize the plasmonic nature of excitations by means of simple indexes that exploit results of first-principle calculations. I will also present some developments in hybrid models towards a real-time description of the molecule-metal nanoparticle systems.