Towards the description of hybrid organic-inorganic Nanosystems: simulating dye-metal interactions and optical properties of the combined system.

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Hybrid organic-inorganic Nanoparticles (HNPs) are very interesting and widely studied materials, for their versatile applications in optoelectronics, biotechnology and medicine, with high potential in biomedical imaging, lab-on-a-chip sensor, gene and drug delivery, and photothermal cancer therapy [1, 2]. However, computing their physico-chemical properties in detail proves to be a challenge. While the nature of the organic component of the HNPs necessitates a full quantum chemical treatment, the size of the inorganic component renders this treatment computationally too expensive to be assessed with a homogeneous technique.

For this reason, hybrid models have been developed combining a QM level treatment and a classical electromagnetism approach, respectively, for molecules and the inorganic nano-structures upon which they are adsorbed [3]. In particular, the inorganic component, usually a metal, is considered as a continuous body, characterized by its own frequency dependent dielectric function (Polarizable Continuum Model, PCM), while excitation energies due to the energy transfer from the molecule to the metal is evaluated exploiting Time Dependent Density Functional Theory (TDDFT).

After proving that the polarization charges distribution, introduced by PCM, well describe the optical properties of bare inorganic Nanoparticles [4], reproducing experimental spectra [5, 6] of bare Gold Nanoparticles using PCM tools, we moved towards the next step: describe the interactions of the organic molecular frame with the Nanoparticles.

This is done at different levels: on one side we are exploiting an electrodynamical model to compute the perturbation due to the presence of the Gold Nanoparticles over the optical properties of organic dyes (either absorption and emission), building up a database of different Nanoparticles, dyes and adsorption positions. The goal is to give the experimentalists a simple tool to get qualitative directions during synthesis to maximize the desired optical properties. On the other side we are trying to reproduce the absorption and scattering properties of the combined system using the same electrodynamic PCM tools of bare Gold Nanoparticles, describing the additional organic layer with different continuous effective models, coming from experimental data or ab-initio calculations.

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