On the Road to the Modeling of Resonance UV/vis Spectroscopic Properties

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Résumé

Upon a resonant excitation by a specific wavelength, the collectively oscillating electrons in the conduction band of a noble metal nanoparticle, *i.e.* localized surface plasmon resonance (LSPR), prompt a strong light absorption in the UV/vis region. The wavelength coincidence of a chromophore with LSPR leads to an enhanced optical response of the system and could facilitate its study at low concentrations [1].
The state-of-the-art modeling of the resonance UV/vis spectroscopic properties relies on a specific hybrid discrete interaction/quantum model (QM/DIM) which describes the chromophore at TDDFT level, in presence of an electrodynamical treatment of the nanoparticle, including electrostatics and polarization of the atoms [2]. However, prior to applying such a complex model, the nanosystem under investigation has to be carefully chosen. Indeed, a resonant coupling between a large inorganic nanoparticle and a small organic chromophore can only occur in specific conditions, thereby necessitating the design of both nanosized systems. We propose here to investigate the optical properties of a new class of versatile chromophores [3] whose first singlet-singlet absorption energy can be tuned to be in resonance with the surface plasmon of a noble metal nanoparticle. At lower size scale, we further show that the coupling between an organic chromophore and an inorganic metal cluster is a methodological challenge. We thus demonstrate how our last developments in DFT can provide some answers to that specific issue [4].

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Mots-Clés: resonance UV/vis spectroscopy, carbenium chromophore, surface, enhanced absorption, range, separated exchange density functionals

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