Evidence for Strong Coupling Phenomena in Molecular Plasmonic Switches: a Density Functional Theory Study

Giulia Giannone[1, 2]
Fabio Della Sala[3], and Stefania D'Agostino[1, 4]

[1] Center for Biomolecular Nanotechnologies @ UNILE – Istituto Italiano di Tecnologia, Via Barsanti, Arnesano, Italy
[2] Department of Mathematics and Physics "E. De Giorgi", University of Salento, Via Arnesano, Lecce, Italy
[3] Istituto per la Microelettronica e Microsistemi – IMM – UOS Lecce, Campus Ecotekne, Via Monteroni, Lecce, Italy
[4] Institute for Materials Science, TU Dresden, 01062 Dresden, Germany

giulia.giannone@iit.it

The recent field of quantum plasmonics offers the possibility to connect the apparently distant worlds of molecular electronics and photonics [1]. This represents nowadays a fascinating challenge for the scientific community, opening crucial topics such as the electro-optical control at the nanoscale of the properties of hybrid metal-molecule systems.

Here, we propose a *Time-Dependent Density Functional Tight-Binding* (TD-DFTB) study with the aim to understand, through a full quantum mechanical approach, the physics of interactions between an optically switchable molecule and a localized surface plasmon excitable in a cluster of a few silver atoms.

In more detail, figure 1 clearly shows how the plasmon excitation of the tetrahedral Ag_{20} cluster can be optically controlled by putting the nanoantenna in proximity of the same molecule (stilbene) in two different spatial conformation (-*trans* and -*cis*). By simply activating the molecular switch, it is possible to move from a small shift of the plasmonic peak registered in the case of -*cis* configuration (see grey curve compared to the orange one) to a couple of well distinguishable peaks resembling, in the -*trans* case, the Rabi-splitting usually appearing in presence of strong-coupling phenomena.

This results in the proof-of concept of a plasmonic switch behavior in which one can activate (-*trans* state) or quench (-*cis* state) the splitting by coupling or decoupling, on demand, the molecular and plasmonics counterparts.

Figures

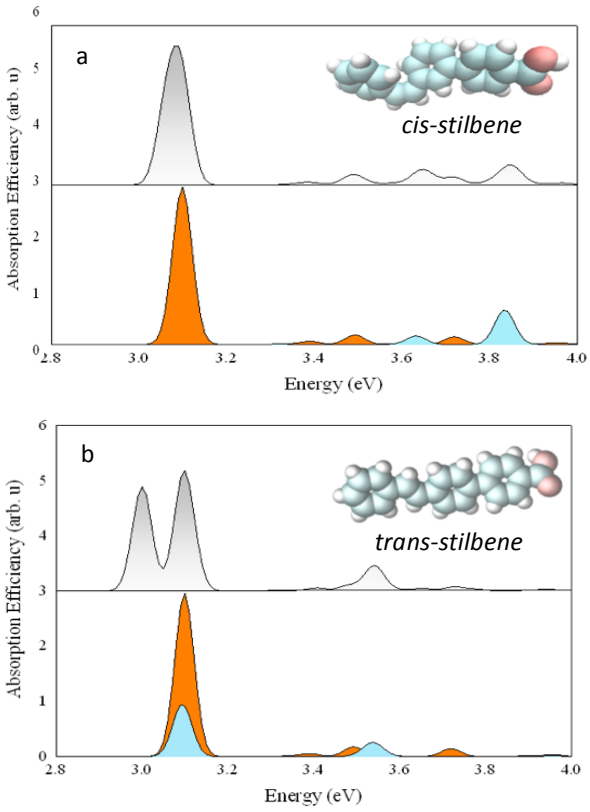

Figure 1.
Optical control of the plasmon excitations of silver nanostructures through the activation of the stilbene *cis*- (panel a) and *trans*- (panel b). The grey filled curves are the TD-DFTB absorption spectra of the whole systems while the orange and light blue filled curves are the TD-DFTB absorption spectra of the Ag_{20} and the molecules, respectively.

References

[1] R. Zia *et al.*, Materials Today **7**, pp. 20-27 (2006).
[2] T. A. Niehaus *et al.*, Phys. Rev. B **63**, 085108 (2001).