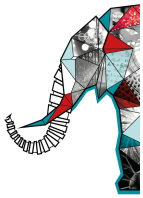
25e Congrès Général de la Société Française de Physique



ID de Contribution: **82** Type: **Poster**

Apports des simulations TDDFT à la réponse plasmonique d'agrégats d'argent

The absorption spectra of silver nanoparticles are characterized by a strong response in the UV-visible range, usually interpreted in the framework of classical optics in terms of plasmon excitations due to the s electrons. Recently, Time-Dependent Density-Functional Theory (TDDFT) calculations have been shown to well reproduce the experimental spectra of metal nanoclusters when using range-separated hybrid (RSH) functionals. This approach gives a new description of the plasmon phenomenon from a quantum point of view. It also gives a framework to investigate the optical properties of small-sized metal clusters for which the classical approaches are no longer valid.

We present new TDDFT simulations of the optical properties of Agn (n=20-147) clusters. In gas phase, the plasmon energies lie between 3.9 and 4.1 eV and varies with size according to the spherical electronic shell model. The plasmon energy is highest for clusters with electrons numbers fully filling states with the lowest radial quantum number (e.g. 1S, 1P, 1D,...). Our results are compared to very recent experimental data measured on clusters embedded in a rare gas matrix or in an oxide matrix. The effects of those matrices over the cluster's optical response are described and evaluated.

[1] C. Yu, R. Schira, H. Brune, B. v. Issendorff, R. Schira, F. Rabilloud, W. Harbich, Nanoscale, 10, 20821-20827 (2018).
[2] R. Schira, F. Rabilloud, J. Phys. Chem C 123, 6205-6212 (2019) ; 122, 27656-27661 (2018).

Choix de session parallèle

5.3 SFO: Metamatériaux, plasmonique

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