Molecular Modelling of metal nanoclusters and nanoparticles: from TDDFT calculations to coarse grained MD simulations

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Metal nanoclusters (NCs) and nanoparticles (NPs) exhibits unique optoelectronic properties that make them very promising nanodevices for a wide range of electronic and biomedical applications.

NCs with diameters less than 2 nm behaves like quantum dots with discrete energy levels and since they present a charging energy greater than the thermal energy they show the so-called Coulomb Blockade effect and can be used to design single electron transistors for future nanoelectronic devices.

Instead, nanoparticles with greater diameters present the plasmonic resonance band and are used in nanomedicine as fluorescent probes for imaging purposes.

It is thus evident that for improving the fields of applications of such systems it is necessary to understand both they optoelectronic properties and how they interact with biological molecules such as blood plasma proteins once they are injected in the body.

This is what we are currently investigating in our research group by means of computational techniques based on quantum mechanical and classical methods.

In order to show some of our recent investigations in the aforementioned fields I have divided my communication in two parts. In the first part, I am going to present some DFT and TD-DFT investigations on several Au, Ag and mixed Au-Ag based nanoclusters protected by organic coatings,[1–4] for which the X-Ray structures and UV-Vis spectra are available in the literature, thus allowing a direct comparison with experimental data.

Instead, in the second part of my presentation I am going to present some findings on the dynamics of the formation of the protein corona around gold nanoparticles with diameters of 5-20 nm that we have done by using coarse-grained molecular dynamics simulations.[5,6]

References:

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