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Computational and Spectroscopic Studies on Metal Nanoparticles

Guest Editor:

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Message from the Guest Editor

Metal nanoparticles represent a bridge between single atoms and bulk materials, presenting peculiar chemical and optical properties. Under irradiation with an appropriate electromagnetic wave, the conduction electrons do not oscillate freely because they are trapped in the nanometric size of the metal particles, which exhibit collective excitations called “localized plasmons”. These latter are needed to promote enhancements for both the Raman signal and the fluorescence emission of molecules adhering to the metal surface, when the exciting radiation wavelengths match those of the plasmon bands. Hence, Raman enhancements up to 10^7 factors are generally observed for molecules adsorbed on silver or gold nanoparticles in the SERS measurements. When, instead, metal particles have sizes below about 2 nm, they do not have metallic properties owing to the existence of discrete electronic energy levels. These particles exhibit a typical quantum size behavior. Different computational approaches can be employed to analyze the spectroscopic properties of these different systems, mainly by adopting the density functional theory and its time-dependent extension.

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Message from the Editor-in-Chief

Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call "nanomaterials". These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal–organic frameworks, membranes, nano-alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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