

THEORETICAL DESIGN OF NEW MATERIALS: ROLE OF PROTECTED NOBLE METAL CLUSTERS FOR BIO-LABELLING AND IMAGING

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Theoretical investigation of the linear and nonlinear optical properties of ligand-protected low nuclearity noble metal clusters will be presented. In this context theoretical approaches for reliable description of two-photon absorption spectra will be addressed. Goal is to design species exhibiting strong one-photon and/or two-photon absorption and emission in the UV-VIS spectral range. We will show that the optical properties can be tuned by creating the appropriate interplay between electronic excitations within the cluster core and selected prototype of ligands. Comparison with available experimental results will be discussed. We conclude that such low nuclearity protected noble metal clusters are promising for bio-labelling and imaging as alternatives to the standard fluorescent probes such as quantum dots or organic dyes.

In addition, we show that the functionalized gold clusters can serve to determine carbonylation sites of proteins responsible for many diseases.