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Theoretical Design of Optoelectronic Properties in TM-Doped Au Nanoalloys

In this work, we employ time-dependent density functional theory (TDDFT) to investigate the optical properties of Au-based hybrid bimetallic nanoalloys, modeling their growth via classical molecular dynamics using the LoDiS package and metal–metal interactions based on the second-moment approximation of the tight-binding scheme (TBSMA). Transition metals (TMs) selected from Au, Ag, Pd, Pt, and Rh are considered, with the analysis constrained to icosahedral seeds—a favorable geometry for such TMs at seed sizes ranging from 0.7 to 3.2 nm. By implementing the complex polarizability TDDFT (PolTDDFT) algorithm, an efficient method able to solve the TDDFT equations for large systems and for a wide energy interval, we explore such systems spectral features as a function of size, shape and chemical composition. Within the same chemical composition the size of the systems determines rather a system has a metallic or molecular- like behavior while their spatial arrangement of atoms governs the emergence of intrinsic chirality, assessed through circular dichroism (CD). Through linear absorption spectra of the analyzed systems we identify the key electronic transitions between ground and excited states, providing preliminary insights into potential collective excitations of conductive electrons, such as plasmons. This last feature is further examined by using the individual component map of oscillator strength (ICM-OS), a diagnostic tool that pinpoints plasmonic excitations based on occupied–virtual state contributions at specific energies. Combined with a fragment-based analysis, this approach allows to discern the role of individual metallic components, revealing whether a particular element promotes those collective electronic behavior in Au or rather their influence suppresses the plasmonic response.

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