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Immobilization effect on optical properties of quantum dots transferred from solution to surfaces probed by nonlinear optical spectroscopy

Quantum dots (QD) constitute a novel generation of fluorescent probes due to their confined size in the 1-10 nm range. In this field, nanosensors sensitivity is of pivotal importance to target biomolecules. We focus here on the optimize grafting of organic ligand-coated CdTe and CdSe/ZnS coreshell type QDs monolayers on glass surfaces to address the environmental problem and cost of nanosensors[1]. QD monolayers samples are pre-characterized by UV-VIS absorption and (Time-resolved) fluorescence emission, evidencing the success of transferring the QD optoelectronic properties from colloidal solution to amine-terminated aliphatic organosilane monolayer-modified glass samples. Moreover, from time-resolved fluorescence spectroscopy, the effect of chemical structure of monolayers are seen from a fast-quenching phenomenon in relation to colloidal QD solution. Afterwards, an advanced surface-specific spectroscopic tool, non-linear optical Two-Colour IR-Visible Sum-Frequency Generation spectroscopy (2C-SFG), is used to probe and evidences the dipolar coupling between QD excitons and their molecular surroundings[2], which improves the nanosensor's detection threshold. This electro-optical coupling (inorganic-organic charge transfer) is modelled through quantum chemical calculations dedicated to spectroscopy. A calculation strategy is optimized in order to properly reproduce the electronic structure of nanostructured systems at semi-empirical and DFT level. Due to the relatively large size of our system, different ones, smaller than ours are modelized, in order to identify possible size effect. The types of interaction involved are characterized using electronic density analysis tools. Semi-empirical methods are used and calibrated in order to perform atomistic simulations on a larger scale to take into account the effects of the chemical environment (solvent, ligands).

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