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Theoretical Study of a Quantum Dot Interacting with Different Functionalizers

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Abstract – To be used as biolabels, the quantum dots need to be connected to biological molecules and this is usually made using organic molecules called functionalizers. The goal of the present work was use quantum chemical calculations to understand the interaction between the cadmium telluride (CdTe) quantum dot with the AMA, AMP, MPS and cysteine functionalizers.

Quantum dots (QD) are semiconductor crystals of nanometric dimensions, which enable the quantum confinement of its electrons [1]. They can be applied as biolabels [2] among other applications. To be used as biolabels, the QDs need to be connected to biological molecules and this is usually made using organic molecules called functionalizers that interact with the surface of the QDs. Despite the importance of the intermolecular interactions between the QDs and the functionalizer molecules to the application of these systems, only a few theoretical works have been developed until now in the attempt of understand these interactions. The goal of the present work was use quantum chemical calculations to understand the interaction between the cadmium telluride (CdTe) QD with different functionalizers used in experimental procedures. We studied the complexation reaction between simplified models of CdTe with the functionalizers mercaptoacetic acid (AMA), mercaptopropionic acid (AMP), trimetoxi mercapto silane (MPS) and cysteine (CYS). The models used to describe the CdTe QD were one Cd^{2+} íon (1Cd), one Cd^{2+} and one Te^{2-} ions (1Cd1Te), four Cd^{2+} ions and tree Te^{2-} íons (4Cd3Te) and four Cd^{2+} and four Te^{2-} íons (4Cd4Te). Initially, we realized the geometry optimizations of the functionalizers and the four CdTe models (1Cd, 1Cd1Te, 4Cd3Te and 4Cd4Te) isolated and then we realized the optimization of the complexes formed between them (functionalizer-QD) with the GAUSSIAN 03 program using the B3LYP/LANL2DZ/6-31G* method. The geometries of some functionalizer-QD complexes optimized by density functional theory are shown in Figure 1. The results indicated that to the 1Cd model the stability increasing order obtained by the complexation energies between the quantum dot and the functionalizer is AMA < AMP < CYS < MPS. These theoretical results corroborate with the initial experimental results obtained by our research group (NIB-UFPE) that the AMA relative stability is smaller than the MPS stability. However, using the 1Cd1Te and 4Cd4Te models we fund a different order. The reason for that discrepancy should be better investigated. We plan to use a better basis set including corrections for the basis set superposition errors to estimate more accurate energy values. We conclude that computational studies can be used to increase the understanding about the interaction between QDs and their functionalizers at a molecular level. As a perspective we intend to improve the QD model using a nanoparticle of 1.6 nm with an ONIOM methodology. We also expect to perform experiments to corroborate the theoretical results.

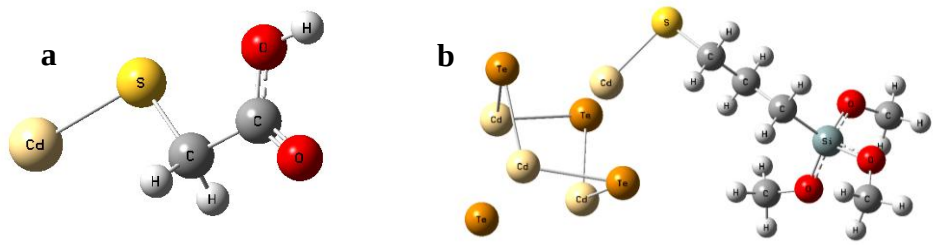

Figure 1: Optimized geometries of the 1Cd-AMA (**a**) and 4Cd4Te-MPS (**b**) complexes.

References

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