Nanocomposites and nanomaterials

Structural and electronic properties of ultrasmall CdS quantum dots doped with transition metals ions

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Ultrasmall semiconductor quantum dots (usQDs), or so-called “magic size” clusters, are very exciting objects to study due to their unique physical properties [1,2]. First of all, they are a broad-band-emitting nanomaterial which can serve in luminescent bio- labeling, sensing, LED technologies, etc. The principle difference between usQDs and “ordinary” QDs is that the single usQD has a large spectral width, comparable with that of a QDs ensemble. Although in the present time there is a significant progress toward the study of such a phenomena, a lot of new questions arise when these usQDs are doped with transition metals ions, what should be another tool to tune their spectral parameters [3]. In the present work, we performed comparative DFT studies of the structural and electronic properties of bare and SCH_3-capped Cd_xS_x with x=15,33 quantum dots both initial and doped with Cu, Mn and Zn ions. Such SCH_3 cap was selected to simulate TGA-stabilised CdS usQDs with a sake of simplicity.

B3LYP/Lanl2dz DFT study were performed to optimize the geometry of the CdS:M, where M is Cu, Mn and Zn, systems and in zero-temperature single-point calculation. In such an approach the HOMO and LUMO energies, projected density of states were calculated to establish the optimal position of the doping ion in the usQD and its influence onto electronic properties.

Ab-initio molecular dynamics was used to establish the presence and the symmetry of crystal structure of CdS usQDs, both bare and SCH_3-capped, and to calculate their room-temperature structural and electronic properties.

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