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CdS/ZnS core shell nanocrystal

J.T Arantes* and G. M. Dalpian

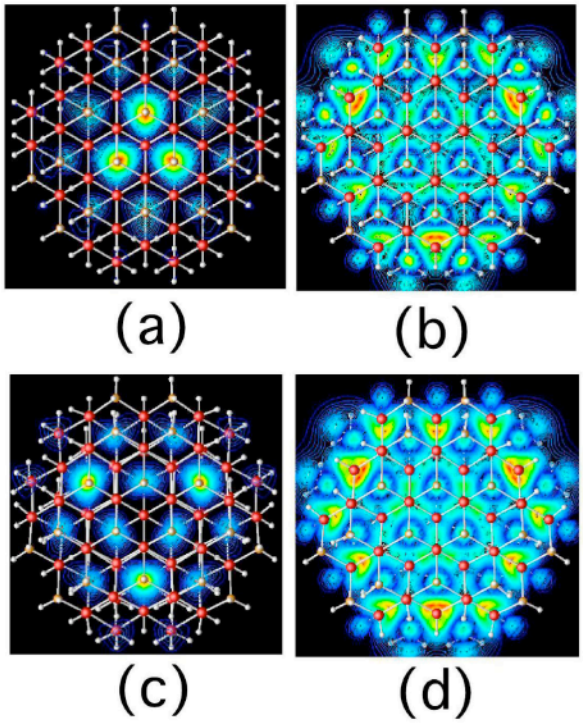
Centro de Ciências Naturais e Humanas, Universidade Federal do ABC, Santo André , SP, Brazil
*e-mail: jjunior@ufabc.edu.br

Abstract – CdS/ZnS and ZnS/CdS core-shell nanocrystals have been studied using real-space ab inition calculations based on the Density Functional Theory and on the pseudopotential method. We have analyzed the effects of quantum confinement on the localization of the band edges of these nanostructures, and we observe that the interface structure is fundamental in order to correctly describe its properties.

Core-Shell semiconductor nanocrystals present improoved properties when compared to standard nanocrystals. Besides of having the possibility of charge separation, they usually blink less than pure nanocrystals, becoming potential candidates for applications such as optoelectronics[1], biolabels and sensing[2], light emitting diodes[3], solar cells[4], spintronics[5,6] and lasers[7]. In a core/shell nanostructured material, the lattice mismatch, the number of shells and the quantum confinement effects will dictate the properties of the nanocrystal. In this work, we show that depending on the difference between the lattice parameter of the materials in the nano heterostructure, the structure of the interface will highly influence the localization of the band edges.

In our work we calculate the electronic structure of CdS/ZnS and ZnS/CdS core shell nanocrystals by using *ab initio theoretical calculations*. We are interested in the effect of quantum confinement and the stress of the interface and the localization of both HOMO and LUMO. Knowing this is important in order to broaden the possible applications of these materials. In figure 1, we show the localization of both HOMO and LUMO (total charge density) in a (001) nanocrystal cross view for the relaxed CdS/ZnS nanocrystal. In a bulk heterostructure with ZnS and CdS materials the system will be a type-I heterostructure with HOMO and LUMO located in the CdS. We can clearly see that this is not the case here.

In this work, we show that the interface structure can change the localization of both HOMO and LUMO. Consequently, using the band offsets extracted from bulk heterostructures or using an effective mass methodology to include quantum confinement effects into these nanostructures is not enough to warrant a good description of these materials.



Charge density for the HOMO and LUMO for the CdS/ZnS core/shell structure using one ZnS shell layer for the nanocrystal fixed in the bulk positions and relaxed. In (a) and (b) we show the HOMO and LUMO respectively for fixed nanocrystal in the bulk lattice parameter. In (c) and (d) we show the HOMO and LUMO respectively for relaxed nanocrystal. The isosurfaces are in e/bohr^3.

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