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Comparative study of the electronic and optical properties of core-shell nanocrystals VANCHO KOCEVSKI, JAN RUSZ, OLLE ERIKSSON, Department of Physics and Astronomy, Uppsala University, Uppsala, D.D. SARMA, Department of Physics and Astronomy, Uppsala University, Uppsala; Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore — The photoluminescence (PL) properties of semiconducting nanocrystals (NCs) can be notably improved by capping the NCs with a shell of another semiconductor, making core-shell structures. Furthermore, their PL properties can be manipulated by changing the core type or the interface between the core and the shell. Here we present a comparative first-principles study of the electronic and optical properties of two different types of core-shell NCs, CdSe/CdS and CdS/ZnS, with four different structural models: pure core, graded core, alloyed interface and graded interface. For the purpose of the study we made NCs with two different diameters, 2.4 nm and 3.0 nm. We show that the electronic and optical properties of the CdS/ZnS NCs are influenced more by the different structural models, compared to the properties of CdSe/CdS NCs. We further looked into the spatial confinement of the HOMO and LUMO wavefunctions (WFs) within the core of the NCs, and the e-h Coulomb interaction energies. We argue that although both types of core-shell NCs have similar confinement of the WFs, the lowering of e-h Coulomb interaction energies, hence increasing the AR lifetimes, in the CdSe/CdS NCs, compared to the CdS/ZnS NCs, is one of the main reasons for the higher quantum yield of the CdSe/CdS NCs.

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