Atomic modeling and simulation of optical properties for Cu-doped ZnSe nanocrystals

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As an important wide band-gap II-VI semiconductor, ZnSe has attracted much attention for its various applications in the visible region, such as blue light-emitting diodes and blue-green diode lasers. As diverse energy states of ZnSe can be tuned by specific conditions of impurities, Cu-doped ZnSe is an interesting quantum dot material. Copper (Cu+ 2) is an excellent dopant for Cu-doped ZnSe synthesized by a cation-exchange scheme. The electronic structures of the ZnSe and ZnSe:Cu were calculated applying the DFT (Density Functional Theory) in the molecular dynamics analysis. The calculated equilibrium lattice constants were compared with respect to different density functionals. For the optimized equilibrium lattice constants agreed with the experimental measurements for ZnSe, the densities of states and energy band structures were further calculated for ZnSe:Cu. By analyzing the partial densities of states for ZnSe:Cu, the contributions of different electron states in different atoms were considered. The calculated results of ZnSe:Cu show the band gap was changed from 2.7eV to lower values reasonably. The calculated optical properties, such as refractive index and absorption spectrum, are discussed qualitatively with respect to different DFT's.