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Investigation of effect of particle size and heterojunction on electron-hole interaction in CdSe and CdSe/ZnS quantum dots JENNIFER ELWARD, JEREMY SCHER, ARINDAM CHAKRABORTY, Syracuse University
— The focus of this work is to explore both the effect of dot size and the effect of heterojunction on the electron-hole (e-h) interaction in nanoparticles. The exciton binding energy (EB), electron-hole recombination probability (P-eh) and average electron-hole separation (R-eh) are important metrics used to quantify the e-h interaction. The form of the wavefunction is critical for accurate representation of these properties. In this work, the explicitly correlated Hartree-Fock (XCHF) and explicitly correlated configuration interaction (XCCI) methods are used. The effect of dot size on e-h interaction was investigated by studying a CdSe quantum dot (QD) system, with diameters ranging from 1-20 nm. The EB and P-eh were found to be strongly dependent on dot size, however, the scaling of each property was distinctly different. The effect of heterojunction was explored by studying a CdSe/ZnS core/shell QD system. The effects of increasing shell thickness, core size and effect of volume versus effect of heterojunction were assessed by computing the EB, P-eh and R-eh. It was found that these properties are also dependent on size, however, the dependence of the CdSe/ZnS core/shell system was markedly different from the CdSe core-only system.

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