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CdSe, CdTe and core-shell CdSe-CdTe nanowires: A density functional study. R. RAMPRASAD, TOM SADOWSKI, University of Connecticut — Semiconductor nanowires (NWs) are attractive in photovoltaic applications due to their ability to support a large number of electron-hole pairs (excitons) and the possibility of enhanced transport of dissociated charge carriers. To facilitate transport along the long axis of the nanowires, efficient charge separation of the exciton is desired. There is evidence suggesting that at a Type II band offset between two semiconductors enables charge separation more easily than in single component systems. The focus of this study is to provide an understanding of the tendency for electron-hole separation in core-shell CdSe-CdTe NWs, which contain a radial Type II band offset. In particular, first principles computational methods have been applied to infinitely long CdSe-CdTe heterostructure NWs in the wurtzite crystal structure over a range of core and shell sizes. The interfacial energy of the nanorods, the band gaps, and the location of the electron and hole states are assessed as a function of the number of CdSe pairs, and core and shell radii. The overlap of the electron and hole wavefunctions, determined to quantify the extent of electron-hole separation, is differentiated with that for single-component CdSe and CdTe nanowires.

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