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Structural and electronic properties of CdS/ZnS core/shell nanowires: A first-principles study HYO SEOK KIM, YONG-HOON KIM[1], Korea Advanced Institute of Science and Technology — Carrying out density functional theory (DFT) calculation, we studied the relative effects of quantum confinement and strain on the electronic structures of II-IV semiconductor compounds with a large lattice-mismatch, CdS and ZnS, in the core/shell nanowire geometry. We considered different core radii and shell thickness of the CdS/ZnS core/shell nanowire, different surface facets, and various defects in the core/shell interface and surface regions. To properly describe the band level alignment at the core/shell boundary, we adopted the self-interaction correction (SIC)-DFT scheme. Implications of our findings in the context of device applications will be also discussed.

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