

Further optical properties of CdX (X¼ S, Te) compounds under quantum dot diameter effect: Ab initio method

Abstract

For energy band calculations, the indirect energy gap ($G_{\Gamma-X}$) is calculated using density functional theory (DFT) of the full potential-linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2K code. The Engel-Vosko generalized gradient approximation (EV-GGA) formalism is used to optimize the corresponding potential for energetic transition and optical properties calculations of CdS and CdTe as a function of quantum dot diameter and is used to test the validity of our model of quantum dot potential. The results are compared with others and showed reasonable agreement.