An ab initio study of the electronic structure and optical properties of $CdS_{1-x}Te_x$ alloys

Abstract

The structural, electronic and optical properties of cubic $CdS_{1-x}Te_x$ alloys, with Te-concentrations varying from 0% up to 100% are investigated. The calculations are based on the total-energy calculations using the full potential-linearized augmented plane wave (FP-LAPW) method. The exchange and correlation potential is treated by the generalized-gradient approximation (GGA) for the total-energy calculations, while for electronic properties in addition to that the Engel-Vosko (EV-GGA) formalism was also applied. The ground state properties for all Te-concentrations are presented. The optical dielectric constant is also determined for both the binary and their related ternary alloys.