Effect of increasing tellurium content on the electronic and optical properties of cadmium selenide telluride alloys CdSe1-xTe x: An ab initio study

A b s t r a c t

An all electron full potential linearized augmented plane wave method, within a framework of GGA (EV-GGA) approach, has been used for an ab initio theoretical study of the effect of increasing tellurium content on the band structure, density of states, and the spectral features of the linear and nonlinear optical susceptibilities of the cadmium-selenide-telluride ternary alloys CdSe1-xTex (x = 0.0, 0.25, 0.5, 0.75 and 1.0). Our calculations show that increasing Te content leads to a decrease in the energy band gap. We find that the band gaps are 0.95 (1.76), 0.89 (1.65), 0.83 (1.56), 0.79 (1.44) and 0.76 (1.31) eV for x = 0.0, 0.25, 0.5, 0.75 and 1.0 in the cubic structure. As these alloys are known to have a wurtzite structure for x less than 0.25, the energy gaps are 0.8 (1.6) eV and 0.7 (1.55) eV for the wurtzite structure (x = 0.0, 0.25) for the GGA (EV-GGA) exchange correlation potentials. This reduction in the energy gaps enhances the functionality of the CdSe 1-xTex alloys, at least for these concentrations, leading to an increase in the effective second-order susceptibility coefficients from 16.75 pm/V (CdSe) to 18.85 pm/V (CdSe0.75Te0.25), 27.23 pm/V (CdSe0.5Te0.5), 32.25 pm/V (CdSe 0.25Te0.75), and 37.70 pm/V (CdTe) for the cubic structure and from 12.65 pm/V (CdSe) to 21.11 pm/V (CdSe0.75Te0.25) in the wurtzite structure. We find a nonlinear relationship between the absorption/emission energies and composition, and a significant enhancement of the electronic properties as a function of tellurium concentration. This variation will help in designing better second-order susceptibility materials by manipulating of the electronic structures of these materials with different compositions to achieve more delocalized atomic bonds.