FP-LAPW investigation of structural, electronic, linear and nonlinear optical properties of $ZnIn_2Te_4$ defect-chalcopyrite

Abstract

A theoretical study of structural, electronic, linear and nonlinear optical properties of $ZnIn_2Te_4$ defect-chalcopyrite is presented using the full-potential linearized augmented plane-wave (FP-LAPW) method. The exchange and correlation potential is treated by the generalized-gradient approximation (GGA). Moreover, the Engel and Vosko GGA formalism (EV-GGA) is also used to improve the band gap results. The lattice parameters (a, c) and the atomic positions (x, y and z) are optimized and found in good agreements with the available experimental data. Our calculations performed for band structure and density of state show that the valence band maximum (VBM) and conduction band minimum (CBM) are located at Γ resulting in a direct energy gap of about 0.89 eV for GGA and 1.20 eV for EV-GGA. The linear optical properties namely, the real and imaginary parts of the dielectric function and the reflectivity spectrum are calculated. This compound possesses a considerable negative birefringence. Based on the density functional theory the nonlinear optical properties are calculated and their spectra are analyzed.