Structural, electronic, linear, and nonlinear optical properties of $ZnCdTe_2$ chalcopyrite

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Abstract :

We report results of first-principles density functional calculations using the full-potential linearized augmented plane wave method. The generalized gradient approximation (GGA) and the Engel–Vosko-GGA (EV-GGA) formalism were used for the exchange–correlation energy to calculate the structural, electronic, linear, and nonlinear optical properties of the chalcopyrite $ZnCdTe_2$ compound. The valence band maximum and the conduction band minimum are located at the Γ-point, resulting in a direct band gap of about 0.71 eV for GGA and 1.29 eV for EV-GGA. The results of bulk properties, such as lattice parameters (a, c, and u), bulk modulus B, and its pressure derivative B' are evaluated. The optical properties of this compound, namely the real and the imaginary parts of the dielectric function, reflectivity, and refractive index, show a considerable anisotropy as a consequence $ZnCdTe_2$ posseses a strong birefringence. In addition, the extinction coefficient, the electron energy loss function, and the nonlinear susceptibility are calculated and their spectra are analyzed.

Keywords : density functional theory; electronic structure; FP-LAPW; generalized gradient approximation; nonlinear optics; optical properties.

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