

First principles investigation of optoelectronic properties of ZnXP_2 ($\text{X} = \text{Si, Ge}$) lattice matched with silicon for tandem solar cells applications using the mBJ exchange potential

H. BANNACER, A. BOUKORTT, S. MESKINE, M. HADJAB, M. I. ZIANE, A. ZAOUI

Abstract: II-IV-V₂ materials are attractive compounds for optoelectronic, photonic and photovoltaic applications due to their valuable ternary chemistry. A primary technological challenge in photovoltaics is to find and develop a lattice matched efficient material to be used in combination with silicon for tandem solar cells. ZnSiP_2 and ZnGeP_2 chalcopyrites are promising semiconductors that could satisfy these criteria. Particularly, ZnSiP_2 is known to have bandgap energy of 2 eV and a lattice mismatch with silicon of 0.5%. In this work, the first principle calculations have been performed to investigate the structural, electronic and optical properties of ZnSiP_2 and ZnGeP_2 in chalcopyrite structure within the Full Potential-Linearized Augmented Plane Wave (FP-LAPW) method based on the Density Functional Theory (DFT) as implemented in WIEN2K code. The local Density approximation (LDA) of Perdew and Wang was used as exchange-correlation potential to calculate the structural properties. Furthermore, the recently modified Becke-Johnson (mBJ) functional of Tran and Blaha was also employed to compute the electronic and optical properties in order to get best values of the band gap energy and some better degree of precision. The complex dielectric function, the complex refractive index, reflectivity, absorption coefficient, and the optical conductivity were calculated to illustrate the linear optical properties of both compounds ZnSiP_2 and ZnGeP_2 . At last, the obtained results indicate that ZnSiP_2 and ZnGeP_2 are attractive materials in optoelectronic devices especially as a lattice matched material with silicon for tandem solar cells applications.

Keywords : FP-LAPW, mBJ, Chalcopyrite, Electronic band structure, Linear optical properties