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First principles investigation of optoelectronic properties ofZnXP2 (X = Si, Ge) lattice matched with silicon for tandemsolar cells applications using the mBJ exchange potential

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Abstract: II-IV-V2 materials are attractive compounds for optoelectronic, photonic and photovoltaicapplications due to their valuable ternary chemistry. A primary technological challengein photovoltaics is to find and develop a lattice matched efficient material to be usedin combination with silicon for tandem solar cells. ZnSiP2 and ZnGeP2 chalcopyrites arepromising semiconductors that could satisfy these criteria. Particularly, ZnSiP2 is known tohave bandgap energy of?2 eV and a lattice mismatch with silicon of 0.5%. In this work, thefirst principle calculations have been performed to investigate the structural, electronic andoptical properties of ZnSiP2 and ZnGeP2 in chalcopyrite structure within the Full Potential-Linearized Augmented Plane Wave (FP-LAPW) method based on the Density FunctionalTheory (DFT) as implemented in WIEN2K code. The local Density approximation (LDA) ofPerdew and Wang was used as exchange-correlation potential to calculate the structuralproprieties. Furthermore, the recently modified Becke-Johnson (mBJ) functional of Tranand Blaha was also employed to compute the electronic and optical properties in order toget best values of the band gap energy and some better degree of precision. The complexdielectric function, the complex refractive index, reflectivity, absorption coefficient, and theoptical conductivity were calculated to illustrate the linear optical properties of both compoundsZnSiP2 and ZnGeP2. At last, the obtained results indicate that ZnSiP2 and ZnGeP2are attractive materials in optoelectronic devices especially as a lattice matched materialwith silicon for tandem solar cells applications.

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