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

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ABSTRACT

II-IV-V_2 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 proprieties. 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.

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1. Introduction

Currently, the civilization and industries are extremely depending on energy. The ordinary resources of energy such as fossil oil and coal are limited by greenhouse gases as a byproduct [1]. Due to greenhouse gases, global warming is expected to increase, as humans add more greenhouse gases [1,2]. So, the solar energy appears to be the most promising to overcome these problems. As the sun is the most abundant, efficient and safe source of energy, photovoltaic solar cells are recently attracting special attention, but, the expensive costs and low efficiency of solar cells have limited their vast use in daily life [3]. However, new suitable materials for photovoltaic and solar cells fabrication technologies have become the object of investigation [3]. For solar cell application, the most important material requirement is that it possesses a high absorption coefficient and thereby should have an optimal direct band gap to absorb the visible light spectrum as well [3–6]. Among the candidate materials we find I-III-VI_2 and II-IV-V_2 chalcopyrites which, recently, have received much attention because of their potential applications in the field of light-emitting diodes, non-linear optical applications, and as a sensitive photovoltaic material in solar cells [7]. Several past studies, show that II-IV-V_2 compounds present higher properties compared to I-III-VI_2 chalcopyrites in terms of hardness, thermo-mechanical, thermo-optical, low scattering losses and non-linearity parameters [8–15]. II-IV-V_2 chalcopyrites are structural analogs to III-V semiconductors, where the group III element is substituted by alternating group II and group IV elements [16,17]. A large number of II-IV-V_2 compounds are formed from abundant and non-toxic elements making them attractive for photovoltaic applications [18]. A continual technological challenge in photovoltaic solar cells is the implementation of an optically lattice matched efficient material to be used in combination with silicon (Si) for tandem cells. $ZnSiP_2$ and $ZnGeP_2$ are among a few materials which are nearly lattice matched with Si and have appropriate band gaps for tandem dual-junction photovoltaics on Si [17]. $ZnSiP_2$ is considered as a promising compound with a band gap of 2.0 eV a lattice mismatch with Si of 5% [17–21]. We have noted that there have been various theoretical and experimental approaches to demonstrate and illustrate the different properties of $ZnSiP_2$ semiconductor [9,22–27]. Further, first principle calculations based on density functional theory (DFT) [28,29] have been used by several researchers to obtain the structural, electronic, optical and magnetic properties of II-IV-V_2 group of semiconductors [4,13,30–33]. Recently, $ZnGeP_2$ has been mainly studied for its capacity as nonlinear optical semiconductor [34]. However, through many years of research and study, there is still not an agreement about the nature of its band structure [34]. In addition, there have been several experimental and theoretical approaches [4,32,35–47] to explain the different physical properties of $ZnGeP_2$ semiconductor [48].

In this work, the structural, electronic and linear optical properties of the both chalcopyrite ternaries $ZnSiP_2$ and $ZnGeP_2$, have been studied, by using the full potential linearized augmented plane wave (FP-LAPW) method [49] based on density functional theory (DFT) [28,29,50]. As a first pace, we have studied the chalcopyrite structure and described the theoretical steps adopted to obtain the structural properties and total energies, where we have used a full total energy minimization for, firstly, obtaining the equilibrium c/a ratio and, secondly, we determined the equilibrium volume, bulk moduli and their derivative for this calculated c/a ratio. The electronic band structure, the density of states and the optical properties will also be computed and discussed in this paper.

2. Computational details

The present calculations are performed using the full-potential linearized augmented plane wave (FP-LAPW) method [51,52] as incorporated in Wien2k package [53].

We consider herein by II-IV-V_2 ternary compounds in body-centered tetragonal chalcopyrite structure (space group $I\bar{4}2d$), shown in Fig. 1, the lattice constant a corresponding to the lattice constant of a cubic zincblende structure, the c/a ratio, and the internal displacement parameter u revealing the distortion of the anion sublattice due to different surroundings. In the ideal structure, $c/a = 2$ and $u = 1/4$ [3,4,9].

Furthermore and in order to achieve energy eigenvalues convergence, the wave functions in the interstitial regions were expanded in plane wave with a cutoff R_{MT} x Kmax equal to 8, where R_{MT} is the minimum radius of the muffin-tin spheres and Kmax gives the magnitude of the largest k vector in the plane wave expansion. Inside the spheres, the valence wave functions were expanded up to $l_{max} = 10$. Intending to keep the same degree of convergence for all the lattice constants, we kept the values of the sphere radii and K_{max} constant over all the considered lattice spacing range. However, the smallest muffin-tin radius in the unit cell R_{MT}, was chosen for the expansion of the wave functions in the interstitial region while the charge density is Fourier expanded up to $G_{max} = 14$ $(Ryd)^{1/2}$. Hence, the muffin tin radii for Zn, Si, Ge and P are chosen to be 2.2, 2.0, 2.2 and 2.0 a.u, consecutively.

The exchange-correlation potential for structural properties was treated using only the local density approximation (LDA) of Perdew and Wang [54]. While for electronic properties, beside, the generalized gradient approximation of Perdew et al. (GGA PBEsol) [55] and the Engel–Vosko-GGA (EV-GGA) formalism [56] we have also applied the modified Becke-Johnson approach (TB-mBJ) proposed recently by Tran and Blaha [57,58] to optimize the corresponding potential for calculating the band structure [59]. The latter has proven to be a promising tool for accurate determination of the fundamental band gaps of wide-band-gap insulators, semiconductors, transition-metal oxides [57,60], half-metallicity [61,62], and doped semiconductors systems [4,57,58,63–66]. Regarding the extraction of optical properties, we also employed the modified Becke-Johnson