

Research Article

First-Principle Calculations to Investigate Structural, Electronic, Elastic, Mechanical, and Optical Properties of K₂CuX (X=As, Sb) Ternary Compounds

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Received 5 July 2022; Accepted 2 September 2022; Published 20 September 2022

Academic Editor: Zhigang Zang

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Efficient materials with good optoelectronic properties are required for the good performance of photovoltaic devices. In this work, we present findings of a theoretical investigation of the structural, electronic, elastic, mechanical, and optical properties of K₂CuX (X = As, Sb) ternary compounds. The computations were carried out by using the density functional theory (DFT) formalism as implemented in the quantum espresso (QE) software package. The calculated lattice constants of 19.1414 a.u (K₂CuAs) and 20.0041 a.u (K₂CuSb) are in agreement with the experimental results from the literature. The materials under study were found to have bandgaps of 1.050 eV (K₂CuAs) and 1.129 eV (K₂CuSb). The valence band was majorly formed by Cu-3d, As-2p, and Cu-4s states while the conduction band was majorly dominated by Cu-5p in K₂CuAs, whereas in K₂CuSb, the valence band was mainly formed by Cu-3d, Cu-4s, and Sb-3p states while the conduction band was majorly formed by Sb-3p and Cu-5p states. The investigated materials were found to be mechanically stable at zero pressure, ductile, and ionic. The optical absorption coefficient curves were found to cover the ultraviolet to visible (UV-Vis) regions, thus making K₂CuAs and K₂CuSb good UV-Vis absorbers hence their suitability for photovoltaic applications.

1. Introduction

Photovoltaic technology depends on various materials for photon-to-electron conversion, which mainly includes organic, inorganic, or organic-inorganic blends [1]. The contemporary photovoltaic industry is currently dominated by the inorganic class with high incidence photon-electron conversion efficiency (IPCE) materials comprising mainly silicon, gallium arsenide, and cadmium telluride, among others [1]. The commercial applicability of these inorganicbased materials in the photovoltaic industries is, however, limited by the high costs and level of purity required during production [2]. Most of these materials, when applied in photovoltaics, work in the principle of light absorption, charge separation, and transport of minority carriers, all happening in the same material [3]. In the recent past, perovskite material has gained traction due to the rapid growth in its conversion efficiency from as low as 3% to the

current 25% [4] in a short span of time. Despite their rapid growth in their efficiency, these types of materials are dogged by the instability of the photovoltaic systems produced by using such materials, and this has begged to cast the search wider [4-7]. The search for alternative classes of materials has led to the realization of cheap and abundant ternary semiconductor compounds [8]. These ternary semiconductor compounds have been found to have excellent electronic as well as optical properties [9]; they also do not require sophisticated technologies when performing thin film deposition since they work on the principle of majority carrier transport, where light absorption and charge separation take place in the absorber, while charge transport takes place in other layers of the optoelectronic device [10]. Among the desirable properties of ternary semiconductor compounds is the considerable wide bandgap range of 1-3 eV [11], which covers the UV-Vis region of the electromagnetic spectrum. This property makes these



FIGURE 1: The orthorhombic crystal structures of (a) K₂CuAs and (b) K₂CuSb ternary compounds.

compounds promising candidates for application in the fields of solar cells, lasers, and photodetectors [12].

Among the ternary semiconductor compounds, ternary compounds adopting the ABC₂-type configuration are most studied due to their wide range of photovoltaic applications [12]. The ABC₂-type ternary compounds comprise chalcogenides with type I-III-VI₂ anions and pnictides with type II-IV-V₂ anions [13]. Experimental studies, as well as theoretical predictions of properties of the ABC₂-type ternary compounds, have been performed for application in the optoelectronic and photovoltaic fields. Among the ABC₂-type ternary compounds, the copper-based ternary compounds have been principally investigated for potential solar cell application [11, 14-18]. Other studies have been carried out on ABC₂-type ternary compounds by replacing the copper element with other elements. For instance, Khan et al. [19] investigated the structural, electronic, and optical properties of ternary CaCN₂ compound by using the DFT, where in their deduction from the study, the results showed that the compound had properties that are suitable for utilization in the photovoltaic applications. Additionally, optical properties of SrSiP₂ and CaSiP₂ compounds by using the DFT approach have been investigated [20]. Elements such as gold, silver, and aluminum, among others, have also been investigated as a replacement for copper for potential optoelectronic and photovoltaic applications [21-42]. Ternary chalcogenides are more promising among the multinary compounds because the majority possess properties such as low toxicity semiconductors and tunable bandgaps allowing improvement of intrinsic properties [43]. In a study for such compounds performed by Regulacio Han, a CuInS₂ compound was studied for application as a light-emitting diode due to its unique properties for bright light emission and nondegradability on thermal exposure. In a different study of ABX compounds, the combination of A = Cu, Ag; B=Zn; and X = Ge, Sn was

TABLE 1: Computed atomic bond lengths within the K_2CuAs and K_2CuSb crystal structures.

Material	Bond	Bond distance (a.u)
	As-K	6.4169
K ₂ CuAs	As-Cu	4.4996
	K-K	7.0447
K ₂ CuSb	Sb-K	6.7652
	Sb-Cu	4.8043
	K-K	7.6135

found suitable for application in photocatalysis [43]. Extensive DFT work of similar compounds is available in the literature, such as $ABiX_2$ and $ABiX_3$ (A = Na, K; X = O, S) and the references therein [44].

ABC₂-type ternary compounds based on potassium elements have been less studied as compared to their copper, silver, gold, and aluminum analogues [45]. Specifically, ternary compounds with K-Cu-X (X=N, P, As, Sb, Bi) formula have been less reported apart from a few exceptions [46–48]. To the best of our knowledge, there are a few experimental reports in the literature on the crystal structure of K-Cu-X (X = As; Sb) [48] hence the motivation for this study. The objective of this work is to investigate the structural, electronic, elastic, mechanical, and optical properties of K₂CuAs and K₂CuSb ternary compounds using the DFT method for potential applications in the photovoltaic field.

2. Computational Details

The structural, electronic, elastic, mechanical, and optical properties of K_2CuAs and K_2CuSb ternary compounds were computed within the DFT [49, 50]. Formalism is implemented in the QE code [51]. The K_2CuAs and K_2CuSb crystal structure input files were downloaded from the materials project database [52, 53]. and the



FIGURE 2: Total energy versus lattice constants computed for (a) K₂CuAs and (b) K₂CuSb compounds.

materials cloud input generator implemented in QE was used to generate the PWscf input files [54] for DFT calculations. The electron-ion interaction was denoted by using the projector augmented-wave function (PAW) method [55]. The Generalized Gradient Approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) [56, 57] was chosen to define the exchange-correlation effect of the electrons. The optimized cutoff energy of 150 Ry and $8 \times 8 \times 8$ Monkhorst-Pack grid for Brillouin zone integration were used. Geometry optimization was performed by computing the total energy per unit cell at several lattice constant values to obtain the ground state structural properties. Based on the optimized lattice constants, the elastic, electronic, and optical properties were calculated.

3. Results and Discussion

3.1. Structural Properties. Both K_2 CuAs and K_2 CuSb ternary compounds adopt an orthorhombic crystal system with the space group Cmcm as reported elsewhere [48]. These crystal structures have K atoms bonded in 4 coordinate geometries to 4 equivalent As and Sb atoms, whereas the Cu atoms are bonded in a linear geometry to 2 equivalent As and Sb atoms [48], as shown in Figure 1.

TABLE 2: Structural properties of K₂CuAs and K₂CuSb ternary compounds.

Structural properties	K ₂ C	CuAs	K ₂ CuSb		
Lattice parameter $a_{\rm o}$ (a.u)	This work 19.1414	Other work 18.9351	This work 20.0041	Other work 19.8421	
Lattice parameter b/a Lattice parameter c/a	0.7545 0.5878		0.7552 0.5933		
Bulk modulus <i>B</i> _o (GPa)	12.5		10.7		
Ground state energy $E_{\rm o}$ (ry)	-1296.22		-1629.72		
Equilibrium volume V_0 (a.u) ³	350	6.64	4002.45		

From Table 1, the As-Cu bond is stronger than the As-K bond in K_2 CuAs, while the Sb-Cu bond is stronger than the Sb-K bond in K_2 CuSb. The K-K bond is the weakest with long bond lengths; this difference is attributed to the fact that the volume per atom tends to increase with the increase in atomic radius and therefore affects crystal lattice basis [13]. The total energy at various lattice constant values is computed and presented in Figure 2.

The computed total energy as a function of lattice constant values was fitted in the Birch-Murnaghan equation of state [58] to get the equilibrium structural



FIGURE 3: The calculated (a) band structure and (b) PDOS of the K₂CuAs ternary compound.

properties. The computed ground state lattice parameters in Table 2 are consistent with the ones reported by Eisenmann et al. [48].

3.2. Electronic Properties. The electronic band structures and projected density of states (PDOSs) of the K₂CuAs and K₂CuSb ternary compounds were computed by using the optimized crystal structures and presented as follows.

The K₂CuAs and K₂CuSb compounds have narrow bandgaps of 1.050 eV and 1.129 eV (see Figures 3(a) and 4(a), respectively. The maxima of the valence bands and the minima of the conduction bands occur at different symmetry points $(Y-\Gamma)$ in the Brillouin zone, implying that K₂CuAs and K₂CuSb ternary compounds are indirect bandgap semiconductors. The projected density of states describes the available states for electrons to occupy when projected on atomic orbitals. By carrying out the projected density of states calculation, we can tell which electronic states (shell (s, p, d, f) and orbital) for a particular atom contribute to the formation of the band edges. Suppose two orbitals lying in the same energy range hybridize, the value of the projected density of states increases. In this way, these orbitals are said to have contributed to the band structure edges. The orbital

contributions to the formation of valence bands and conduction bands are described by the PDOS in the energy region -3.5 eV to 5 eV. As illustrated in Figure 3(b), the upper valence band in the region -1.4 to the Fermi level was majorly formed by As-2p and Cu-3d with a small contribution from the other states while the middle valence band in the energy region -2.6 eV to -1.5 eV was majorly formed by Cu-3d with few contributions from the other states. The lower valence band in the energy region -3 eV to -3.4 eV was formed mainly by As-2p, Cu-3d, and Cu-4s, whereas the conduction band was majorly formed by Cu-5p and As-1s with little contribution from the other states. In the case of the K_2 CuSb compound (Figure 4(b)), the valence band was majorly formed by the Cu-3d, Sb-3p, and Cu-4s orbitals, while the conduction band was majorly formed by the Cu-5p and Sb-3p orbitals.

3.3. Elastic and Mechanical Properties. The K₂CuAs and K₂CuSb ternary compounds adopt an orthorhombic crystal structure featuring 9 independent elastic constants [59] given as C_{11} , C_{12} , C_{13} , C_{22} , C_{23} , C_{33} , C_{44} , C_{55} , and C_{66} . The necessary and sufficient conditions for elastic stability of the orthorhombic crystal system [59, 60] are given as



FIGURE 4: The calculated (a) band structure and (b) PDOS of the K₂CuSb ternary compound.

TABLE 3: Computed elastic constants C_{ij} (GPa) of K₂CuAs and K₂CuSb compounds.

Compound	C11	C ₁₂	C ₁₃	C ₂₂	C ₂₃	C ₃₃	C ₄₄	C55	C ₆₆
K ₂ CuAs	45.13	8.23	5.70	38.93	20.15	34.40	22.00	7.09	4.68
K ₂ CuSb	37.27	8.88	4.68	31.96	18.30	27.42	18.75	6.64	3.09

TABLE 4: Voigt-Reuss-Hill approximations of bulk modulus B (GPa), Young's modulus E (GPa), shear modulus G (GPa), Pugh's ratio B/G, and Poisson's ratio n.

Compound	В	E	G	B/G	n
K ₂ CuAs	20.59	26.94	10.55	1.95	0.27
K ₂ CuSb	17.56	21.28	8.24	2.13	0.29

$$\begin{cases} C_{11} > 0; C_{11}C_{22} > C_{12}^2, \\ C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23}, \\ -C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 > 0, \\ C_{44} > 0; C_{55} > 0; C_{66} > 0. \end{cases}$$
(1)

The computed elastic constants in Table 3 satisfy the conditions for elastic stability of the orthorhombic system; thus, the K_2CuAs and K_2CuSb ternary compounds are mechanically stable. Other mechanical properties are shown in Table 4.

Bulk modulus measures the resistance against volume change resulting from applied external pressure [61]. Large B



FIGURE 5: Calculated optical properties of K2CuAs and K2CuSb ternary compounds.

value predicts hard materials; thus, from the computed values of the bulk modulus, both K₂CuAs and K₂CuSb are not hard materials. Additionally, the bond lengths of the crystal structures are correlated to the size of the B. The shorter the bond lengths, the larger the B value [61]. From the structural properties, the obtained bond lengths in K₂CuAs are shorter than those in the K₂CuSb crystal structure thus the higher value of B in the K₂CuAs compound. The ductile (ionic) and brittle (covalent) nature of materials is determined by using Pugh's ratio B/G and Poisson's ratio, *n* [62]. The restriction for brittleness is B/G < 1.75; otherwise, the material is said to be ductile [63].

Poisson's ratio n = 0.1, 0.25, and 0.33 for pure covalent, ionic, and metallic bonds, respectively, [64]. Thus, we can conclude that K₂CuAs and K₂CuSb ternary compounds are ductile and strongly dominated by ionic character. These findings are in agreement with the other reports in the literature for compounds with similar stoichiometry [47]. The stiffness of a material is determined by applying Young's modulus value [65]. The higher the value of *E*, the stiffer the material [65]; therefore, K₂CuAs compound is stiffer than K₂CuSb.

3.4. Optical Properties. To explore the prospect of any material for solar cell and optoelectronic applications, an

investigation of the materials' frequency response of various optical constants to the incident photon radiation is key [66]. A complex dielectric wave function describes the electron response in a material [67], and it is described in the form of an equation as

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega), \qquad (2)$$

where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ refer to the real and imaginary parts of the complex dielectric wave function. All the other optical constants including the absorption coefficients $\alpha(\omega)$, refractive index $n(\omega)$, extinction coefficient K(ω), reflectivity R (ω), and energy loss function $L(\omega)$ presented in Figure 5 are computed by using the equations presented as follows [41], [63, 68, 69]:

$$\alpha(\omega) = \sqrt{2}\omega \left(\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right)^{1/2},$$

$$n(\omega) = \left(\frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} + \varepsilon_1(\omega)}{2}\right)^{1/2},$$

$$K(\omega) = \left(\frac{\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)}{2}\right)^{1/2},$$
(3)

$$L(\omega) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)},$$
$$R(\omega) = \frac{(n-1)^2 + K^2}{(n+1)^2 + K^2}.$$

The imaginary part of the dielectric wave function describes the photon absorption in crystalline materials [61]. The peaks in $\varepsilon_2(\omega)$ curves result from the electronic transitions from the valence to the conduction bands. The absorption onsets in $\varepsilon_2(\omega)$ curves refer to the materials bandgaps which lie within the visible region, <3.1 eV for K₂CuAs and K₂CuSb compounds, an implication of strong interband transitions. This makes K2CuAs and K₂CuSb promising candidates for solar cell applications [41]. Additionally, narrow bandgaps facilitate faster electron transitions as opposed to wide bandgaps [61]. The key feature of the $\varepsilon_1(\omega)$ curve is $\varepsilon_1(Energy = 0)$, also referred to as the static value [70]. This static value is correlated to the material's refractive index as $n = \sqrt{(\varepsilon_1(0))}$. Starting from Energy = 0, the $\varepsilon_1(\omega)$ plot attained major peaks at low energy regions, 1.786 eV and 1.652 eV for K₂CuAs and K₂CuSb, respectively. The photon transmission persisted until the $\varepsilon_1(\omega)$ values became negative at energy regions 5.681-9.173 eV. At this energy region, the incident photon radiations are assumed to be fully attenuated [71] and the compounds assert a metallic behaviour [72]. The calculated refractive indices for K₂CuAs and K₂CuSb were 2.49 and 2.55, respectively. The major refractive index peaks reside within the visible region. The optical absorption coefficients of K₂CuAs and K₂CuSb compounds cover the UV-Vis regions in the

range of 2.82-11.71 eV; this demonstrates that these compounds can be utilized for photovoltaic applications. The materials' surface behaviour and energy loss by fast electrons entering a medium are determined by reflectivity and energy loss function, respectively [41]. The main peaks of the reflectivity curves were observed in the regions 2.217-5.345 eV. The reflectivity decreased beyond this region. There was no significant absorption in the visible regions, as depicted in the loss spectrum. The major absorption peak occurred at higher energy regions >10 eV. The optical properties' results obtained in this work are in agreement with the results obtained previously on the related materials [46, 47].

4. Conclusions

In summary, we have studied the structural, electronic, elastic, mechanical, and optical properties of K₂CuAs and K₂CuSb ternary compounds by using the DFT method as implemented in the QE package. Equilibrium lattice constants of 19.1414 and 20.0041 a.u were obtained for K2CuAs and K₂CuSb, respectively. The bandgaps obtained were 1.050 eV and 1.129 eV for K₂CuAs and K₂CuSb, respectively. The formation of the valence band was primarily by Cu-3d, As-2p, and Cu-4s states, while the conduction band was majorly formed by Cu-5p and As-1s states in K2CuAs whereas, in K₂CuSb, the valence band was majorly formed by Cu-3d, Cu-4s, and Sb-3p states while the conduction band was mainly formed by Sb-3p and Cu-5p states. Both K₂CuAs and K₂CuSb were found to be mechanically stable at zero pressure, ductile, and ionic, thus their potentiality for resilient materials application. The calculated bandgaps, high refractive indices, high absorption coefficients, and wide energy coverage of the absorption coefficients spectra, mainly in the UV-Vis regions of the electromagnetic spectrum, make K₂CuAs and K₂CuSb ternary compounds suitable for photovoltaic applications.

Data Availability

The source files and raw data supporting the conclusions in this paper will be assessed upon request from the authors.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

This work was supported by the Partnership for Skills in Applied Sciences, Engineering and Technology (PASET)— Regional Scholarship Innovation Fund (RSIF) and ISP Sweden through the KEN02 grant. RSIF is also gratefully thanked for grant number RSIF-RA-015. The authors acknowledge the Centre for High-Performance Computing, CHPC, Cape Town, and RSA for HPC resources.

Supplementary Materials

The results and conclusions of this work are supported by a supplementary file submitted along with the manuscript. The File comprises the K₂CuX (X = As, Sb) crystal structure data, the pseudopotentials, Plane Wave selfconsistent field (PWscf) input files, output files for structural properties, output files for elastic and mechanical properties as well as the Equations used for calculating optical properties. Also, the references to K₂CuX (X = As, Sb) source files are provided. Supplementary Materials (*Supplementary Materials*)

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