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Ab initio Calculation of $CuSbSe_2$ in Bulk and Monolayer for Solar Cell and Infrared Optoelectronic Applications

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Abstract: *The production of efficient, less toxic and low-cost solar cell devices is still faced with numerous challenges. However, copper antimony selenide ($CuSbSe_2$) appears to be the more promising material due to cost effectiveness, ease of availability and less toxicity. Therefore, the exploration of the potential of this composite requires, comprehensive analysis of its structural, electronic and optical properties. To accomplish this purpose, first-principles calculations employing the development of correction terms for the van der Waals interaction has been implemented in this study. Results obtained from structural properties calculations indicated that the role of van der Waals (vdW) interactions on structural properties of layered materials can be predicted from theoretical bases because results obtained for the lattice parameters using vdW on top of PBE were in good correlation with experimental results. The electronic properties investigations gave values for the electronic band structures, partial and total densities of states. Indirect band gap was observed for bulk $CuSbSe_2$ with band gap value of 0.83 eV, which was also in agreement with experiment result. By reducing the dimension from bulk to monolayer a direct band gap smaller than that of bulk form was obtained, indicating that $CuSbSe_2$ is suitable for solar cell and near infrared optoelectronic applications. The optical gap of $CuSbSe_2$ in bulk and monolayer structure was found to be 0.83 and 0.21 eV respectively. Therefore, $CuSbSe_2$ can absorb photons, whose energy lies between that of the near infrared to visible light frequency. The study confirmed the importance of van der Waals interaction in predicting, structural, electronic and optical properties of layered materials. Analysis of optical parameters suggested that a device fabricated from these materials can be operated on a wide range of energy scale including solar cells, optical communications and biomedical imaging.*

Keywords: *$CuSbSe_2$, DFT, vdW, Solar cell, Optical Communication.*

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1.0 Introduction

Nowadays, a drastic rise in the population and globalization has increased the demand for sustainable and clean energy sources than ever (Quaschning, 2019) . To deal with global energy demand, the harvest of solar energy through photovoltaic (PV) technology is among the best options because the resource is natural, renewable and environmentally friendly (Pillot, Muselli, Poggi, & Dias, 2019; Zoungrana & Çakmakci, 2021). This has made the discovery and application of new energy sources. In 1954, Chapin *et al*, have pioneered a silicon-based p-n junction device with a power conversion efficiency of 6% (Chapin, Fuller, & Pearson, 1954). Since then, the application of crystalline silicon in the solar energy industry is widely accepted and currently dominates the PV research area (Sharma & Chandel, 2016). The utilization of silicon-based PV modules remained dominant for decades until the energy challenge has been disputed in mankind due to the rise in population and globalization (Zou *et al*., 2019). Hence, a necessity in finding photoactive materials with better performance, lifetime, abundant availability, cost-effective and environment-friendly are demanded to meet mankind's needs (Javed *et al*., 2020).

Although many absorber materials have been established for solar cell technology. However, the achievement of low-cost, non-toxic, abundant and efficient solar cell materials is still a challenging job for researchers (Pitchaiya *et al*., 2020). Therefore, the dire requirement for more efficient, low-cost, and non-toxic optoelectronic devices has led to the increased focus on a range of different source materials along with the development of methodologies to characterize these materials (Nair, Patel, & Gohel, 2020; Radzwan, Ahmed, Shaari, Lawal, & Ng, 2017; Radzwan *et al*., 2020). Conversely, $CuSbSe_2$ semiconductor material with the optical band gap of 1.05 eV (Zhou *et al*., 2009) is considered among the most promising candidates for solar cell application owing to its abundant, less toxic and low cost. Thus, this material could be a better replacement for the scarce, toxic, and expensive materials being used as an absorber layer in solar cells such as CdTe and CIGS. Although comprehensive studies have been done on $CuSbSe_2$ material, the indirect bandgap nature of $CuSbSe_2$ limited its application for solar cells. In order to overcome the indirect band gap nature of $CuSbSe_2$ material in bulk form. One of the methods is reducing the dimension of the materials. Studies have shown that by reducing the dimension of semiconductor materials, the nature of bandgap changes from indirect to direct (Ramasamy, Gupta, Sims, *et al*., 2015; Ramasamy, Sims, Butler, & Gupta, 2014).

The $CuSbSe_2$ compound, which belongs to the orthorhombic system with Pnma space groups, has two dimension (2-D) double layered structure with six-membered hetero rings of Sb_2CuSe_3 and $SbCu_2Se_3$, where the Cu atom has distorted tetrahedral coordination with four Se atoms and the Sb atom is coordinated to three Se atoms. $CuSbSe_2$ crystal shows potential applications for photovoltaic devices, solar cells and near infrared photodetector due to its narrow bandgap of 1.05 eV. Generally, there are two possible ways of analysis in the field of condensed matter physics. One way is to characterize and analyze materials experimentally for their properties. However, in some instances, it is not easy to furnish experiments at some conditions for characterization. The second possibility is to solve many-body problems by solving quantum mechanical equations, this method also takes a long time. Conversely, with the advancement in computer processing

technology, computational methods have gained enormous attention in recent years and can perform analysis on physical properties of materials accurately within a short period. Approaches based on computational physics can calculate the physical properties of materials precisely and sometimes replace experimental methods which are difficult to execute under standard conditions. Density functional theory leads to an ab-initio method (First-principles approach), which has opened a new era in material research. In DFT calculations exchange and correlation functions are important for overall energy estimation. It was found to be more reliable and provides better results concerning the electronic structure calculations in designing and modeling new materials and tuning their properties without prior experimental knowledge. This feature of DFT has brought new insight into the investigation and education field. In this paper we theoretically investigated electronic and optical properties of bulk and monolayer of $CuSbSe_2$ in detail, using density functional theory (DFT) calculations as implemented in the Quantum Espresso simulation package (Giannozzi *et al*., 2009).

2.0 Computational Details

The flow of the methodology is starting from the optimization procedures with input parameters, after the structures are optimized then the structural properties are obtained. Next, calculations involving electronic and optical properties are conducted from the optimized structures. In structural and electronic properties, all of the calculations were carried out by the DFT computational code called Quantum Espresso (Giannozzi *et al*., 2009). Expansion of wave function is dealt with by applying plane-wave basis approach to grasp all the interactions that may occur in crystal structures (Lawal & Shaari, 2016). We have treated the core orbital as frozen by applying the pseudopotential approach. All of the structures have been optimized by suppressing the geometry through SCF convergence until each structure reach 0.0001eV/atom, and then the structure was allowed to relax fully. For structural relaxation, the electron-electron are treated with generalized gradient approximation (GGA) in the form of Perdew–Berke–Erzndof (PBE) functionals and local density approximation (LDA). In addition to the semi-local GGA and LDA, we implemented vdW-DF approach for the exchange-correlation functional to take into account the effect of van der Waals (vdW) interaction.

For electronic properties calculations of the bulk form, the electron-electron and van der Waals effects were treated with generalized gradient approximation (GGA) in the form of Perdew–Berke–Erzndof (PBE) functionals and vdW approach. Plane-wave kinetic energy cut-offs of 50 Ry and charge density of 260 Ry were found to be sufficient for calculating electronic band structures. The irreducible Brillouin zone was sampled with a set of 11×11×11 Monkhorst-Pack grid to generate k-points and a denser value of 16×16×16 was used for the density of states using a technique known as Hermite-Gaussian smearing. On the other hand, for monolayer band structure calculations. A 11×11×1 k-point mesh grid was used for the integration of the Brillouin zone (BZ). To avoid unwanted interactions between the nearest layers, a large vacuum layer of 30 Å was used so that periodic images and the layer can be treated independently as can be seen in Fig. 1 (b). A plane-wave basis set with kinetic energy cutoffs of 50 Ry was used to expand the electron wave functions and 250 Ry for charge density. Also, the atomic positions are relaxed until Hellmann-Feynman forces acting on each ion is less than 10^{-3} eV/Å. For optical properties calculation, the spectra of the optical absorption have been investigated at the level PBE-GGA functional level. All of the optical calculations are realized within Yambo (Marini, Hogan, Grüning, & Varsano, 2009) computational code.

3.0 Results and Discussion

3.1 Convergence Test Results of $CuSbSe_2$

In any first principles calculations, it is of paramount importance to perform a convergence test calculation before commencing the actual calculation. Fig. 1(a) shows that from $20\,Ry$ to $40\,Ry$ the total energy varies significantly with the kinetic energy cut-off. The kinetic energy cut-off remains almost constant from $40\,Ry$. This means, that the kinetic energy cut-off converged from $40\,Ry$. Therefore, in our calculations, $50\,Ry$ is used as the plane wave basis set for the kinetic energy cut-off. The variations of the total energy for the k-points grids is shown in Fig. 1(b). The total energy changes considerably with the k-points indicating a well-converged value at particular points. However, the total energy remains almost steady at $6 \times 6 \times 6$ k-points. As such, $11 \times 11 \times 11$ k-points have been used as optimized k-points for $CuSbSe_2$.

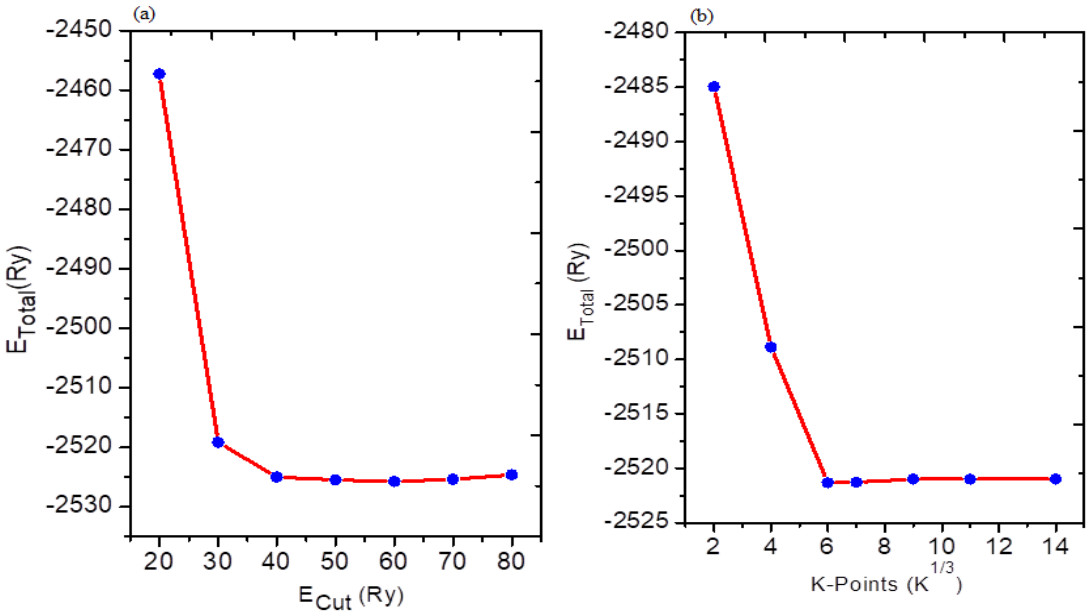

Fig 1: (a) The convergence of total energy concerning the kinetic energy cut-off. (b) The convergence of the total energy for the k-points grids.

3.2 Structural Properties of $CuSbSe_2$ in Bulk and Monolayer

The structural parameters of both bulk and monolayer of $CuSbSe_2$ have been relaxed for accurate predictions of electronic and optical absorptions. Generally, structural relaxation is the first step in any first-principles calculation to avoid some errors for precise predictions of fundamental band gap and optical spectra. Structural relaxation is a process whereby atomic coordinates and cell parameters are adjusted so that the total energy of the structure is minimized to obtain a stable structure. Complete optimization processes will provide a stable geometry. In structural properties, all of the calculations were carried out by the developed DFT computational code Quantum Espresso. Generally, structural relaxation is the first step in any first-principles calculation to avoid some errors for accurate predictions of other quantities like bandgap and optical absorptions. Bulk $CuSbSe_2$ has orthorhombic with space group Pnma (No. 62) and has four Cu, four Sb, and eight Se atoms in the unit cell (see Fig. 2 (a)). The optimized distance between the Sb atoms of neighbouring atomic layers was found to be 2.11 Å for bulk $CuSbSe_2$ and this value is in reasonable agreement with the experimental value of 2.14 Å (Ramasamy, Gupta, Palchoudhury, Ivanov, & Gupta, 2015). Table 1 presents the fully relaxed lattice

parameters of $CuSbSe_2$ in orthorhombic crystal structure along with experimental results. The calculated lattice parameters with van der Waals (vdW) correction are consistent with the available experimental results. From our first-principles calculations, we observed that PBE-GGA tends to overestimate the lattice parameter *c* while LDA underestimates the lattice parameter *c*. However, lattice parameters and interlayer distance *a*, *b* and *c* calculated with inclusion of the vdW corrections are interestingly closer to the experimental results. Our results indicated that the inclusion of vdW correction in layer materials is needed for accurate prediction of reliable lattice parameters, as it gives the best matching with experimental results.

Table 1: Calculated and experimental lattice constants of $CuSbSe_2$

Ref.	XC	*a* (Å)	*b* (Å)	*c* (Å)
Present work	LDA	5.98	3.86	13.67
	PBE-GGA	6.474	3.971	14.754
	PBE-GGA+ vdW-$DF^{C09}x$	6.395	3.944	15.322
Experiment (Imamov, Pinsker, & Ivchenko, 1965)		6.4	3.95	15.33

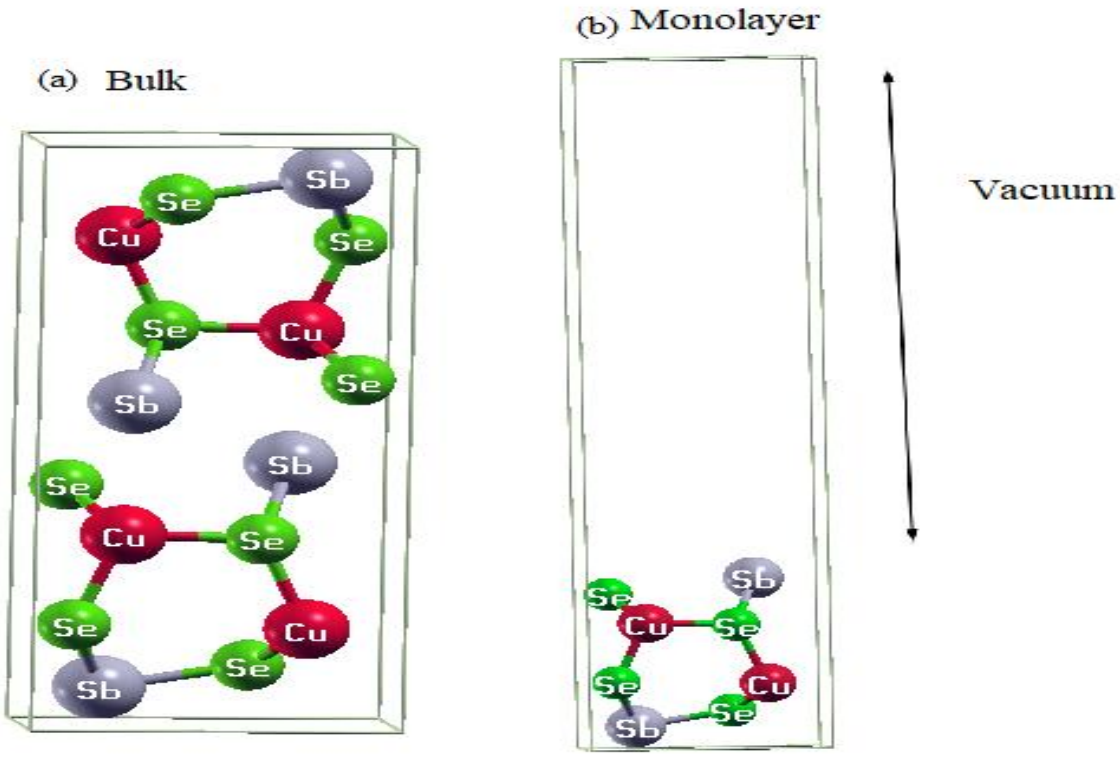

Fig. 2: (a) Optimized bulk crystal structure of $CuSbSe_2$ (a) Bulk (b) Monolayer structures

3.3 Electronic Properties of $CuSbSe_2$ in Bulk and Monolayer

Electronic properties investigations of $CuSbSe_2$ in bulk and monolayer structures covers the band structure, Total density of state (DOS) and partial density of state (PDOS). The main purpose of the ground state, electronic band structure, DOS and PDOS calculations in this work is to obtain the KS eigenvalues and eigenfunctions as well as useful information about the electronic properties of the concerned materials. By using a fully optimized structure, we have investigated the band structure of the bulk and monolayer of $CuSbSe_2$ material. The band structure calculations of bulk and monolayer of $CuSbSe_2$ have been computed using DFT within PBE approximation plus van der Waals correlation. The band structures were calculated along with the high-symmetry directions of the irreducible Brillouin zone (BZ) $\Gamma \rightarrow X \rightarrow U \rightarrow Z \rightarrow \Gamma \rightarrow Y \rightarrow S \rightarrow R \rightarrow T$ in the k-space and the Fermi energy level is set at 0 eV. The calculated energy band structure of bulk $CuSbSe_2$ with GGA-PBE plus van der Waals corrections are displayed in Fig. 3. For band structure calculations, the energy separation between the valance band maximum and conduction band minimum was found to be 0.83 eV and this value is reasonably in agreement with experimental results (Zhou *et al*., 2009). Our result is better than the previous first principles approach due to the effects of vdW correction (Alsaleh, Singh, & Schwingenschlögl, 2016; Maeda & Wada, 2015; Xue *et al*., 2015). Electronic band structure results indicated that van der Waals corrections are important for predicting band gap value for layered material. Also, from the same figure, the conduction band minimum occurred at Y point while the valance band maximum is located in between R and T, indicating that bulk $CuSbSe_2$ has an indirect bandgap which is in agreement with previous theoretical and experimental findings (Maeda & Wada, 2015; Xue *et al*., 2015). As the structures transfer from bulk to monolayer phase, the dimension considered reduces from three to two dimensions (2D) as can be seen in Fig. 2 (b). In the case of $CuSbSe_2$ monolayer, the energy separation between the valance band maximum and the conduction band minimum was found to be 0.22 eV. The calculated band gap value of monolayer is smaller than that of the bulk form. This trend is consistent with previous studies (Alsaleh *et al*., 2016; Ramasamy, Gupta, Palchoudhury, *et al*., 2015; Ramasamy *et al*., 2014). Furthermore, the conduction band minimum and the valance band maximum occurred at Γ point, indicating that $CuSbSe_2$ monolayer has a direct bandgap. The nature of the bandgap of $CuSbSe_2$ monolayer agreed well with previous studies (Alsaleh *et al*., 2016; Ramasamy, Gupta, Palchoudhury, *et al*., 2015; Ramasamy *et al*., 2014). The reduction of the bandgap of $CuSbSe_2$ monolayer is different from MoS2 in which the bandgap increases by reducing the dimension to 2D (monolayer). The increase in the bandgap of MoS_2 monolayer is due to the presence of S atoms at the van der Waals gap whereas the positions of Mo atoms are the same in monolayer and bulk form. As a consequence, in the case of MoS_2 monolayer, the S atoms dominated the valence band maximum is shifted to lower energy but not Mo dominated the conduction band edge. Conversely, the position of Sb and S atoms are located at the van der Waals gap in the case of $CuSbS_2$. Therefore, a similar effect does not appear in the case of $CuSbSe_2$ monolayer. The calculated bandgap values of $CuSbSe_2$ for both bulk and monolayer together with previous theoretical and experimental results are listed in Table 2.

To further elaborate on the origin and nature of $CuSbSe_2$ band gap, we have also studied the total and partial densities of states (TDOS and PDOS). The results of TDOS and PDOS of $CuSbSe_2$ in bulk and monolayer are shown in Fig. 4(a) and (b) respectively.

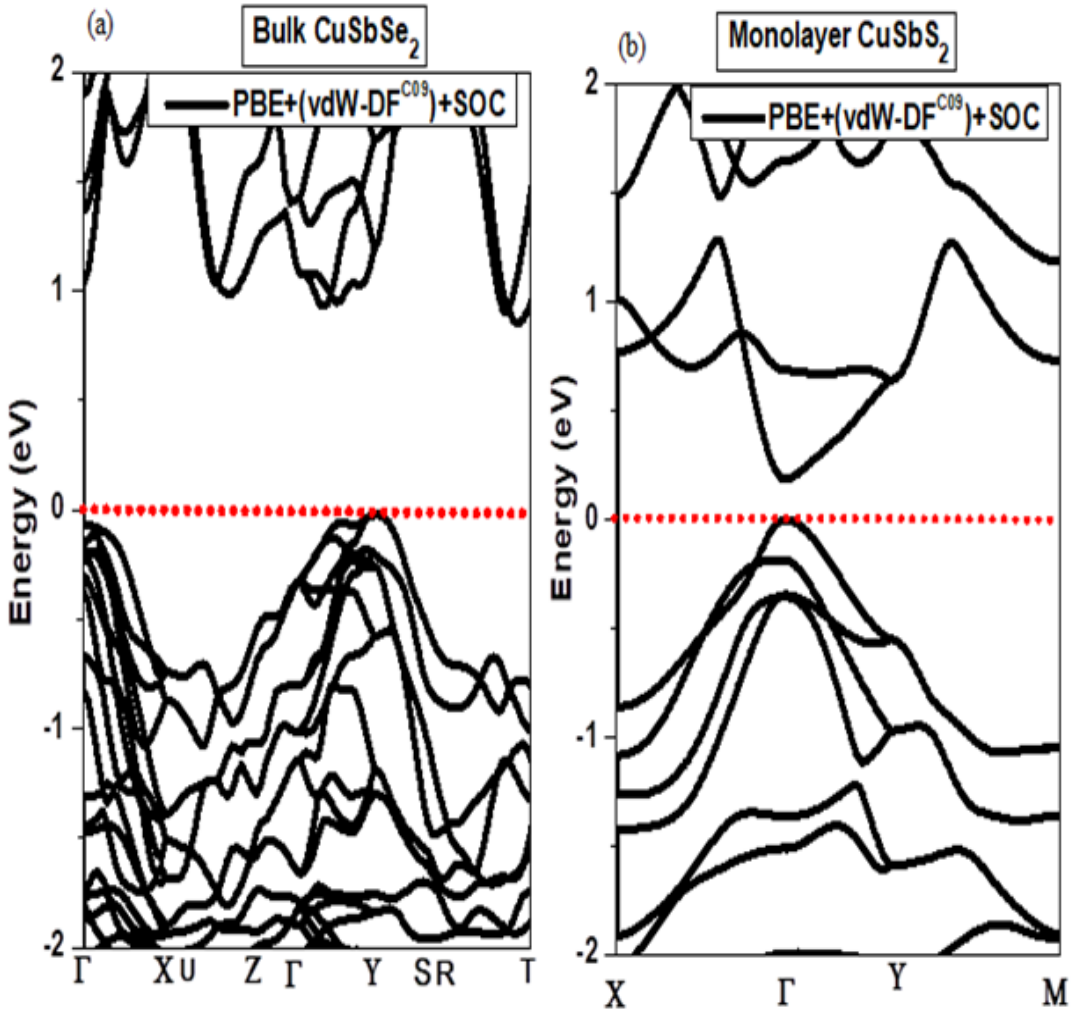

Fig. 3: Electronic band structure of $CuSbSe_2$ in (a) Bulk and (b) monolayer structures

Table 2 Calculated and experimental band gap value of $CuSbS_2$ in bulk form and monolayer

Method	Bandgap value (eV)	
	Bulk	**Monolayer**
PBE+vdW	0.83	0.22
PBE (Alsaleh *et al*., 2016)	0.49	0.15
TB-mBJ (Alsaleh *et al*., 2016)	0.78	0.21
HSE06 (Maeda & Wada, 2015)	0.66	-
Exp. (Zhou *et al*., 2009)	1.05	-

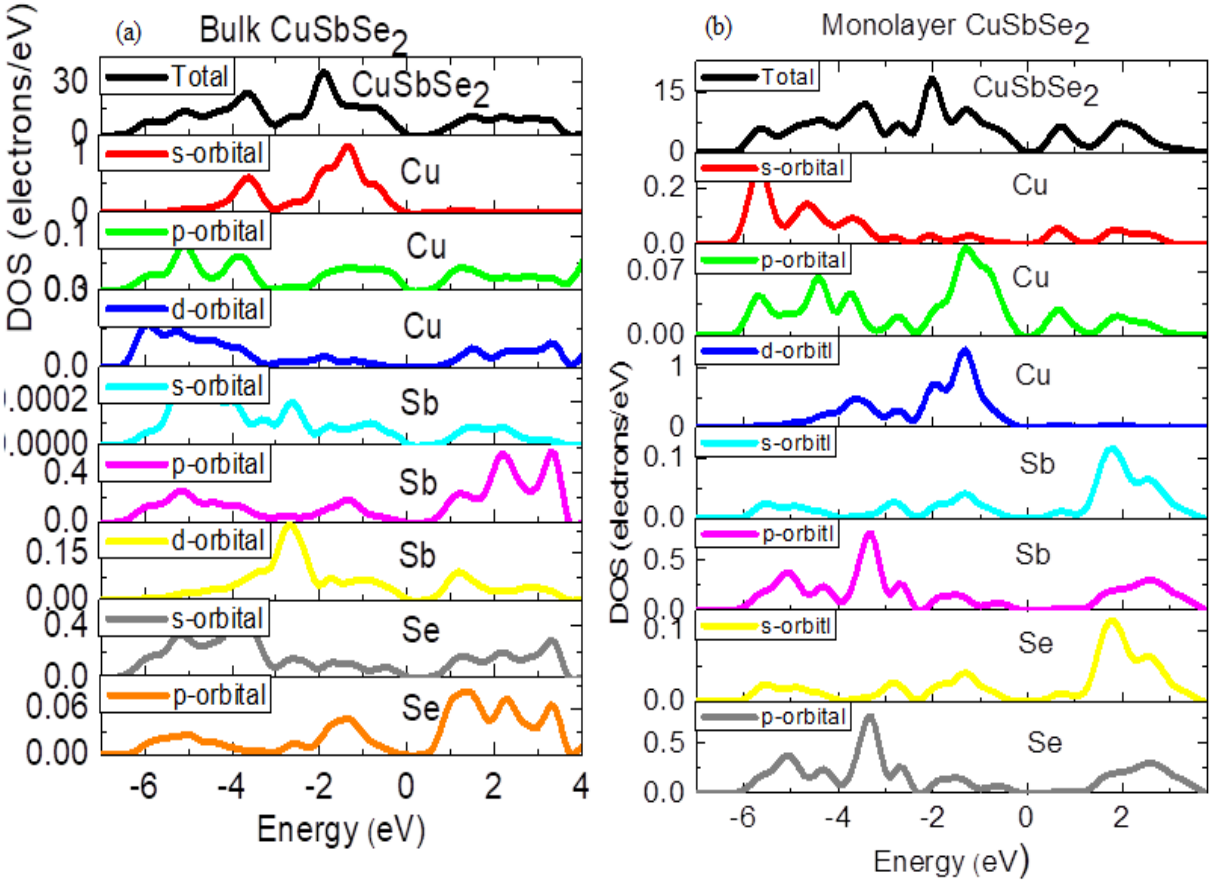

Fig. 0.: Total and partial DOS of $CuSbSe_2$ in (a) Bulk and (b) monolayer structures

The TDOS shows three distinct structures of electronic states separated from each other by energy gaps.

From Fig. 4 (a), we found that the p-orbitals of Sb and Se atoms are energetically contributing the most to the conduction bands. While in the case of monolayer s-orbitals of Sb and Se contributed the most to the conduction bands. For bulk structure, s-orbital of Cu atoms was found to contribute the most to the upper part of the occupied valence band nearly the Fermi level. While the middle of the valence band is principally due to d-orbital of Sb atoms for bulk structure and p-orbitals of Sb and Se atoms in the case of the monolayer.

3.4 Optical Properties of $CuSbSe_2$ in Bulk and Monolayer

This section provides the results of optical absorption of bulk and monolayer of $CuSbSe_2$ with the inclusion of van der Waals correction which is examined for the first time. Optical absorptions investigation of materials is crucial to get insight into their characteristics for optoelectronic applications. From the comprehensive literature review, it is found that the exploration of the optical features relating to the $CuSbSe_2$ monolayer is scarcely studied. To complete the study on optoelectronic properties in addition to electronic properties, comprehensive studies are presented on the optical absorptions of the say compounds by employing DFT+RPA approach (Random-phase approximation (RPA)) as implemented in Yambo simulation package (Marini *et al*., 2009; Onida, Reining, & Rubio, 2002).

Generally, macroscopic dielectric functions describes the response of the material to electromagnetic waves and are also useful in the prediction of the band structure configuration (Lawal *et al*., 2021; Radzwan *et al*., 2020). Fig. 5 presents the results of the macroscopic dielectric function (imaginary part) of $CuSbSe_2$ calculated with the electric field of the incoming light polarized along the x-direction. The macroscopic dielectric function (imaginary part) is a gauge that describes what an electric field like a light wave does to the condensed-matter system (Lawal *et al*., 2019). The imaginary part of the macroscopic dielectric function is a quantity that provides useful information on how much material is capable to absorb photon energy (Lawal, Shaari, Ahmed, & Taura, 2018; Mazumder *et al*., 2021). Material is transparent when the imaginary part of the dielectric function is zero, but becomes nonzero as soon as absorption begins. The calculated $\varepsilon_2(\omega)$ shows that the first critical point which sometimes called optical gap occur at 0.82 eV for $CuSbSe_2$ bulk form and 0.22 eV in the case of monolayer. On the other hand, we found explicit improvement in the optical absorption in the case of monolayer structure when compared with the bulk form. Our result pointed out that reducing dimension of layered materials increases the optical options and this trend is in good agreement with other findings (Bafekry *et al*., 2021; Guo, Xiao, Wang, & Zhang, 2019; Ni, Quintana, Jia, & Song, 2021; Sun, Martinez, & Wang, 2016). Optical gap of 0.22 eV and strong absorption in the near ifrared to visible light wavelenghts for monolayer structure, suggest that $CuSbSe_2$ semiconductor material is a promising candidate for solar cells and near infrared opto-electronic applications such as biomedical imaging, gas sensing and optical communication.

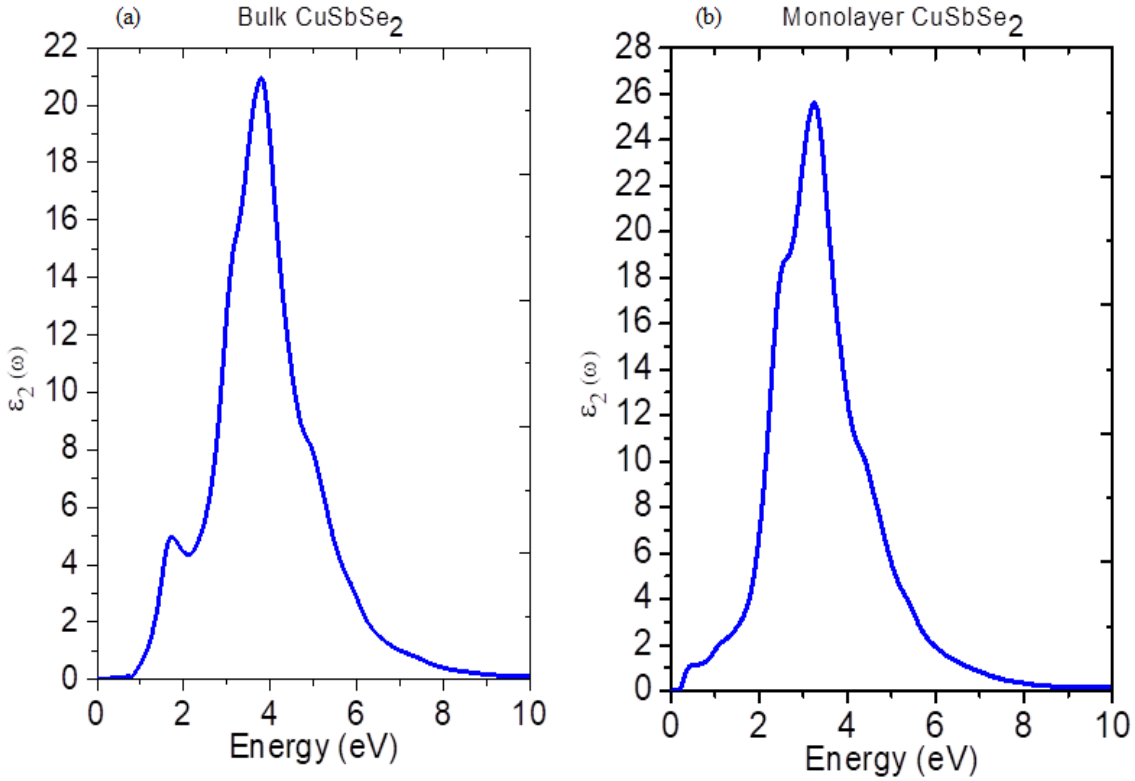

Fig. 5: Imaginary part of the dielectric function of (a) Bulk and (b) monolayer structures

4.0 Conclusions

In this study, we have provided a consistent theoretical description of the structural, electronic and optical properties of $CuSbSe_2$ in bulk and monolayer form using the first principles approach within the DFT framework. Structural properties calculations reveal the role of van der Waals (vdW) interactions on structural properties of layered materials, as the obtained results of lattice parameters using vdW on top of PBE are almost the same as experimental results. The electronic properties investigation involves electronic band structures, partial and total densities of states. The underestimated band gaps within bare PBE were found to be sufficiently improved by adding van der Waals interactions. Indirect bandgap nature is revealed for bulk $CuSbSe_2$ with a bandgap value of 0.83 eV and this value is close to experimental results. By reducing the dimension from bulk to monolayer a direct bandgap smaller than that of bulk form was obtained and this value makes $CuSbSe_2$ suitable for solar cell and near infrared optoelectronic applications. In addition to electronic properties, we studied optical properties $CuSbSe_2$. The optical gap of $CuSbSe_2$ in bulk and monolayer structures was found to be 0.83 and 0.21 eV respectively. These values reveal that $CuSbSe_2$ can absorb photons within near infrared to visible light frequency. Moreover, our calculations revealed the importance of van der Waals interaction in predicting, structural, electronic and optical properties of layered materials. Analysis of optical parameters suggested that a device fabricated from these materials can be operated on a wide range of energy scale including solar cells, optical communications, biomedical imaging and remote sensing.

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Conflict of Interest

The authors declared no conflict of interest. All authors took part in analyzing the results, proofreading and effecting all corrections. All authors read and approved the final manuscript