Highly anisotropic electronic and mechanical properties of monolayer and bilayer As$_2$S$_3$

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ABSTRACT

Two-dimensional (2D) material with high anisotropy as well as robust stability would inspire significant interest in the new-generation electronic and optomechanical field, especially for directional memories, synaptic, neuromorphic and polarization-sensitive photodetector devices. Recently, 2D As$_2$S$_3$ was successfully exfoliated in experiments (Šíksins et al., 2019) and was demonstrated to be stable in the ambient. Herein, by using first principles method, we further systematically predicted its angular-dependent electronic and mechanical properties. Specifically, the angle-resolved effective mass of carriers, carrier mobility, three dimensional band structure, stress–strain relationships, as well as the angle-dependent mechanical properties are investigated. Our results show that 2D As$_2$S$_3$ owns a high anisotropic nature both electronically and mechanically. We found that, due to the large anisotropic charge distributions, 2D single (bilayer) As$_2$S$_3$ has shown a value of 3.15 (3.32) in Young’s modulus ratio along two axes. These values are much greater than the corresponding 2D black phosphorous of 2 (Tao et al., 2015), which is experimentally confirmed the largest one up to date. Our findings provide an valuable avenue to realize the flexible orientation-dependent nano-devices.

1. Introduction

Many materials are anisotropic and even inhomogeneous owning to the tunable formation and composition of their constituents and elements. Currently, large amount of two-dimensional (2D) materials including graphene [3,4], h-BN [5], transition metal dichalcogenides [6,7] are found to be isotropic. During the past years, some 2D structures were demonstrated with limited anisotropy, Such as SnSe [8], and atomically thin tellurium [9,10]. Besides, although black phosphorus [11] was found to be a highly anisotropic 2D material, the weak stability seriously constrain its practical applications. Most glasses and polymers are examples of isotropic materials, which have been widely used in the packaging industry, medical equipment, and even home tableware. On the contrary, the properties of anisotropic materials are direction-dependent, which usually consists of asymmetric crystalline structures. Furthermore, artificial anisotropic single crystals (metamaterials) are also highly desired as developing technology, such as selective fluorescence DNA sensors [12], anisotropic synaptic devices for neuromorphic applications [13], anisotropic nanoelectronics with multifunctional directional memories in the 2D limit [14], digital inverters [15], and even polarization-sensitive broadband photodetectors [16].

Recently, low-symmetry monolayer and few-layer materials have appeared on the stage owing to the unique orientation-dependent properties that are not easily obtained in the usual isotropic and symmetric 2D materials [17–21,2]. In these anisotropic 2D materials, the electronic, optical, thermal, piezoelectric, and even ferroelectric properties are direction-dependent, which would open up more potential to selectively harness the physical properties of 2D materials-based nano-devices [22,15,23,14,24]. At present, 2D black phosphorus (BP) was reported having a large value of $E_t/E_s = 2$ in Young’s modulus [2,25]. BP, yet, has a fatal disadvantage that is unstable in the ambient conditions, which severely constrains its potential applications [26].

Past year, free-standing 2D As$_2$S$_3$ with robust atmospheric stability was exfoliated successfully in the experiment by Šíksins et al. [1] and...
they have also systematically studied the anisotropic optical properties such as Raman spectroscopy, resonance frequency analysis using laser interferometry [1]. However, both the mechanical and electronic anisotropic character of 2D As$_2$S$_3$ is still unclear yet. Is the anisotropy of a single (bilayer) layer greater than that of a multi-layer in As$_2$S$_3$? How does the anisotropy of monolayer and bilayer As$_2$S$_3$ compare to the well-known BP?

Herein, we have systematically explored the anisotropic properties of 2D As$_2$S$_3$ using first-principle methods, mainly focusing on the electronic and mechanical properties. Furthermore, we have elaborately analyzed the angle-resolved effective mass of holes and electrons, angle-resolved Young’s modulus, Poisson’s ratio and Shear modulus of monolayer and bilayer As$_2$S$_3$. The calculated anisotropic factor of monolayer and bilayer As$_2$S$_3$ are 3.15 and 3.32 respectively, which are quite larger than the renowned BP with an anisotropic ratio of 2. Our studies will provide a more comprehensive understanding and insights into the potential applications of 2D As$_2$S$_3$ in orientation-dependent nanoscience and nanotechnology.

2. Computational methods

The optimization of structures and static self-consistent energy calculations were conducted using the PBE functional [27]. We optimized materials and calculated band structures in vasp code [28,29]. The energy cutoff is 400 eV. We use a $4 \times 12 \times 1$ Monkhorst–Pack k-point to sample the reciprocal space. The energy and force on each atoms criterion are $10^{-5}$ eV and 0.02 eV/Å. Van der Waals (vdW) dynamical correlations was also considered by the DFT-D2 method of Grimme [30], a correction to the conventional Kohn–Sham DFT energy. A vacuum thickness with 20 Åwas used. To describe a more accurate band structure, we used HSE06 [31]. The angle-resolved effective mass of holes and electrons, angle-resolved mechanical properties were performed using VASPKIT code [32].

![Fig. 1. (a)(b) Top and side views of the monolayer and bilayer 2D As$_2$S$_3$ in a $2 \times 2$ supercell. The primitive cell of monolayer As$_2$S$_3$ is indicated by a solid black rectangle. According to the different hinged deformation, the As—S—As bond angles can be classified into two types (A and B), shown in (a) and (b). (c), (g) and (h) depict the Bader charge distribution for monolayer, bilayer and three layer As$_2$S$_3$, respectively. (d)-(f) (except for (h)) describe the electron localization function (ELF) for monolayer (above) and bilayer (below) As$_2$S$_3$, separately. (d) and (e) are the 3D ELF and the iso-surface value in the side views of ELF is 0.59. The Miller indexes for top views and side views are (0 0 1/2) and (0 1/2 0). The blue and red colors in (c) and (g) represent gaining and losing electrons, and the number of transferred electrons are characterised by the depth of colors. The maximum value of obtaining and losing electrons are shown in (c) and (g). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image-url)
and bilayer, respectively. By comparing the depth of red or blue color in Figs. 1(c) and (g), it is also obvious that the number of transferred electrons in the bilayer As$_3$S$_3$ is much more than that in monolayer As$_3$S$_2$. The different amount of electrons transfer originates from the Van der Waals interaction between the two sub-layers in the bilayer structure. In order to get a clear picture of the change, we further calculated the Bader charge for three-layer As$_3$S$_3$, as shown in Fig. 1(h). As expected, the Bader charge feature is very similar to that of the bilayer case. The average transfer electrons from the arsenic atom to the sulphur atom are 0.43 e, which is approximate to that of the bilayer. Besides, the different color distributions of Bader charge along $\vec{a}$ and $\vec{b}$ direction imply the anisotropy of electronic properties in 2D As$_3$S$_3$.

Electron localization function (ELF) is another tool to investigate the bonding nature between two atoms [37]. It is a three-dimensional function with a value ranging from 0 that indicates a low electron density localization and metallic ionic bonds to 1 that implies strong covalent bonding or lone pair electrons. The calculated ELF for monolayer As$_3$S$_3$ are shown in Figs. 1(e) and 1(f). The result shows that ELF of sulfur atoms is larger than that of arsenic atoms, indicating a large anisotropic charge distribution of monolayer As$_3$S$_3$. Figs. 1(j) and 1(k) also depict a similar charge distribution of bilayer As$_3$S$_3$ with the monolayer As$_3$S$_3$. Furthermore, the strong electron localization locates between sulfur and arsenic atoms, indicating the dominant role of covalent bonding in both monolayer and bilayer As$_3$S$_3$.

The Bader charge and ELF can be further explained by the different electronegativity of sulfur (2.58) and arsenic (2.18) atoms. Therefore, sulfur atoms tend to gain more electrons than arsenic atoms due to a larger electronegativity. This covalent bond mechanism in bilayer As$_3$S$_3$ is stronger than the monolayer As$_3$S$_3$, which can be verified in Figs. 1(c) and 1(l). What is more, Figs. 1(f) and 1(k) display the different electron densities in the 2D plane, no matter in monolayer and bilayer As$_3$S$_3$. This outcome demonstrates that electrons are more continuous and dense in the $\vec{a}$ axis compared with the $\vec{b}$ axis, suggesting a large anisotropic charge distribution for monolayer and bilayer As$_3$S$_3$. This special electron behavior will lead to the anisotropic properties of As$_3$S$_3$. We will discuss it in the following sections.

3.2. Anisotropic electronic transport properties

Next, we study the electronic properties of both monolayer and bilayer As$_3$S$_3$. The calculated band structures are shown in Figs. 2(a) and 2(b), indicating indirect semiconductors for monolayer and bilayer As$_3$S$_3$. For monolayer, the CBM is occurred at the $\Gamma$ point while the VBM lies between the $\Gamma$ and Y point (0 1/2 0), marked as $\Delta$ in the -2(a). In the case of the bilayer, the location of CBM changes little but the VBM is transformed to the S point (1/2 1/2 0), due to the weak vdW interaction. Based on the DFT-PBE calculations, the monolayer As$_3$S$_3$ has an indirect band gap of 2.17 eV, and the bilayer is 1.97 eV. This is consistent with the physical picture that usually monolayer material has a larger band gap than that of the few-layer material [38].

Considering the fundamental bandgap of As$_3$S$_3$ is underestimated in DFT-PBE calculations, we have resorted to the HSE06. The calculated HSE06 band gaps for monolayer and bilayer As$_3$S$_3$ are 3.11 and 2.91 eV, respectively. Our monolayer HSE06 band gap is 0.16 eV smaller than the previous work [35] since we used a much dense $k$ point to do the calculation. Note that the locations of CBM and VBM are the same as their results [35]. It is also found that the HSE06 method does not change not only the shape of the band structures of monolayer and bilayer As$_3$S$_3$ but also for the positions of CBM and VBM (band edges). Besides, the bands shown in Figs. 2(a) at CBM along $\Gamma$–X direction are more non-dispersive than that of $\Gamma$–Y direction, resulting in a smaller electron effective mass along $\Gamma$–X direction. In the case of the bilayer, the band edge along $\Gamma$–X direction is much flatter than that of $\Gamma$–Y direction, thus, leading to a larger electron effective mass in $\Gamma$–X direction. As for the VBM, a similar discussion can be done but is omitted for simplicity. The carrier effective masses at band edges for monolayer and bilayer As$_3$S$_3$ along two different directions are listed in Table 1. These results indicate strong electronic anisotropy for monolayer and bilayer As$_3$S$_3$, which can be explained by the anisotropic crystal structure, as shown in Fig. 1(a), the lattice constant in $\vec{b}$ direction is much smaller than that of $\vec{a}$ direction. Besides, as discussed above based on the Bader charge results, the charge distribution is not uniform, thus would induce the anisotropic electronic properties as well. Therefore, we need more quantitative study of electronic transport properties for As$_3$S$_3$ systems in the following.

Besides, we also show the atomic projected density of states (PDOS) as well as the charge density distributions of VBM and CBM based on the HSE06 level for monolayer in Fig. 1 bilayer in Figs. 3(e), 3(g) and 3(f). Evidently, the PDOS for monolayer and bilayer As$_3$S$_3$ show that the VBM is mainly dominated by the p orbital of sulfur atoms. On the contrary, the

![Fig. 2. Electronic band structures of (a) monolayer and (b) bilayer 2D As$_3$S$_3$ using the DFT-PBE (dashed green) and DFT-HSE06 (solid red) functionals. The insertion in (a) is the Brillouin zone of 2D As$_3$S$_3$. The high-symmetry k are: S(0.5 0.5 0), X(0.5 0 0), $\Gamma$(0 0 0), $\Delta$(0.26 0) and Y(0 0.5 0). $E_F$ is the Fermi level. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)](image)
In order to get a clear picture of the bonding and antibonding nature in CBM is equally contributed by the strong anisotropic electronic transport properties. The effective mass much more dispersive than that of the VBM band edges, again indicating obvious anisotropic nature at the CBM and VBM. CBM band edges are along the radial direction at intervals of 10 degrees to calculate the band orientation-dependent effective mass, a uniform electron momentum along (a, b, c) direction. During the process of different electronic bands according to the Eq. (1) will result in quantitative effective mass of carriers in different directions. The orientation-dependent effective masses of holes and electrons are depicted in Figs. 4(b) and 4(c) for monolayer and Figs. 4(e) and 4(f) for bilayer As$_2$S$_3$ respectively. Obviously, the effective mass of electrons along $\bar{a}$ direction is much smaller than that of in the $\bar{b}$ direction. As for the holes, an opposite trend is found and the anisotropic nature of holes is much stronger than the electrons. These significantly anisotropic transport properties could be beneficial to the separation of electrons and holes which is highly desired in the photovoltaic field [41]. Furthermore, the bilayer As$_2$S$_3$ has a larger anisotropic effective masses of holes and electrons compared with the monolayer situation, which will lead to asymmetric transport properties, such as the Seebeck coefficient and electric conductivity and finally potentially enhance the thermoelectric performance [42,43].

In order to give out a clearer understanding about the anisotropy of transport properties, it is necessary to calculate the mobility of electrons and holes in the 2D As$_2$S$_3$. Based on the deformation potentials theory proposed by J.Bardeen and W.Shockley [44], the mobility of 2D mate-
where the $e$, $\hbar$, $C$, $D$, $k_B$, $T$, and $m^*$ are the charge of an electron, reduce Planck’s constant, elastic modulus of 2D As$_2$S$_3$, Boltzmann constant, thermodynamic temperature, the effective mass of carriers, respectively. 

$m_d$ is the average effective mass of electron or hole determined by $m_d = \sqrt{m_x^*m_y^*}$ and $E_1$ denotes the deformation potential constant of the VBM for hole and CBM for electron, calculated by $E_1 = \Delta E / (\Delta l / l_0)$. Here, $l_0$ and $\Delta l$ are the lattice constant and the deformation of $l_0$, separately, and the change step of deformation is 0.5% within a range from $-2\%$ to $+2\%$. The mobility as well as other related quantities are summarized in Table 1.

The mobility of electron(hole) for monolayer As$_2$S$_3$ in x and y direction is predicted to be 253.11 (10.85) and 163.78 (13.74) cm$^2$ V$^{-1}$ s$^{-1}$, respectively. As for the bilayer As$_2$S$_3$, the corresponding mobility is 81.91 (6.61) and 66.23 (26.07) cm$^2$ V$^{-1}$ s$^{-1}$, separately. The results show an obviously anisotropic carrier mobility for 2D As$_2$S$_3$.

Besides, the mobility of holes are much smaller than electrons in both monolayer and bilayer structure, which is beneficial for carrier separation required in the photovoltaic and photocatalytic fields.

### 3.3. Anisotropic mechanical properties

The mechanical properties of a material are those properties that involve a response to an applied strain, which has wide applications [46–48]. The calculated stress–strain curves of monolayer and bilayer As$_2$S$_3$ are shown in Fig. 5, which starts a linear function before the loaded strain is lower than 5%. Above 5%, monolayer and bilayer As$_2$S$_3$ enter nonlinear (anharmonic) regions, which are consistent with the previous work [35]. Young’s modulus $E$ is the slope in the stress–strain curve locating in the linear region [47]. By fitting calculation, we obtained the elastic modulus for monolayer (bilayer) are 45.4 (85.1) GPa,
and 11.3 (27.4) GPa along with the $x$ (a) and $y$ (b) directions, respectively. Due to the rectangle crystals of monolayer and bilayer As$_2$S$_3$, the mechanical properties along with $x$-direction can decouple with the $y$-direction, which further increases the anisotropic mechanical properties of As$_2$S$_3$ systems. This is completely verified by the Figs. 5(a) for monolayer and 5(b) for bilayer As$_2$S$_3$.

For a 2D material, the relationship between the stress $\sigma$, the in-plane elastic constants tensor $C_{ij}$ ($i,j=1,2,6$) and strain $\varepsilon$ can be correlated based on the Hooke’s law under the in-plane stress condition [49,47]

$$
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{xy}
\end{bmatrix} =
\begin{bmatrix}
C_{11} & C_{12} & 0 \\
C_{12} & C_{22} & 0 \\
0 & 0 & C_{66}
\end{bmatrix}
\begin{bmatrix}
\varepsilon_{xx} \\
\varepsilon_{yy} \\
\varepsilon_{xy}
\end{bmatrix}
$$

(3)

where we use the standard Voigt notation which simplifies the tensor notation into the matrix notation, such as $1-xx$, $2-yy$, and $6-xy$ [50]. Besides, since the rectangle crystals of monolayer and bilayer As$_2$S$_3$, the elastic constants can be calculated as

$$
E_i = \frac{1}{2} C_{11} \varepsilon_{ii}^2 + \frac{1}{2} C_{12} \varepsilon_{ii}^2 + C_{11} \varepsilon_{1i} \varepsilon_{2i} + 2 C_{66} \varepsilon_{6i}^2
$$

(4)

where $E_i$ is the strain energy and the tensile strain is defined as $\varepsilon = \frac{L_0 - L}{L_0}$ ($i = x, y$), $L_0$ and $L$ are the strained and unstrained lattice constants along with $x$- or $y$-directions, respectively. To capture the physics, we select the $\varepsilon_1$ ($i = 1, 2, 6$) ranging from the $-2\%$ to $2\%$ with an increment of $0.5\%$ to calculate the strain energies under different strains for all strained structures, including monolayer and bilayer As$_2$S$_3$. Thus the elastic constants can be obtained by fitting the Eq. (4).

To intuitively investigate the mechanical anisotropy of As$_2$S$_3$ systems, we calculate the orientation-dependent Young’s modulus $E(\theta)$, Poisson’s ratio $\nu(\theta)$, and Shear modulus $G(\theta)$ based on [51,52]

$$
E^{-1} = S_{11} \cos^4 \theta + S_{12} \sin^2 \theta + 2 S_{16} \cos \theta \sin \theta + 2 S_{26} \cos \theta \sin \theta + (2 S_{12} + S_{66}) \cos \theta \sin \theta
$$

(5)

and

\[ -\nu(\theta)/E(\theta) = A + B \cos(4\theta + \psi), \]

where

\[ A = (|S_{11} + S_{22} - S_{16}|/2 + 3 |S_{12}|)/4, \]

\[ B = |(S_{26} - S_{16})^2 + (|S_{12} - (S_{11} + S_{22} - S_{66})/2|^2)/4, \]

\[ \tan\psi_i = \frac{S_{26} - S_{16}}{S_{12} - (S_{11} + S_{22} - S_{66})/2}; \]

\[ 1/4G(\theta) = C + D \cos(4\theta + \psi), \]

where

\[ C = (S_{11} + S_{22} - 2S_{12} - S_{66})/8; \]

\[ D = \sqrt{(S_{66} + 3 S_{12} - S_{11} - S_{22})^2/4 + (S_{16} - S_{26})^2}/4; \]

\[ \tan\psi_i = \frac{2(S_{16} - S_{26})}{(S_{66} + 3 S_{12} - S_{11} - S_{22})}. \]

(6)

(7)

(8)

(9)

(10)

(11)

(12)

(13)

in which $\theta \in [0, 2\pi]$ is the conventional angle that starts from the $+x$ axis corresponding to the $\theta = 0$. In the experiment, the data of mechanical property sometimes are compliance constants that have a straightforward relation with elastic tensors: $S_{ij}=C_{ij}^{-1}$. Our calculated results are presented in Figs. 6(a) and 6(c) for monolayer and Figs. 6(d) and 6(f) for bilayer As$_2$S$_3$.

At first glance, for bilayer As$_2$S$_3$, both Young’s modulus $E$ and Poisson’s ratio $\nu$ decrease to a minimum value then increase as a function of orientation. The maximum and minimum values of $E$ for bilayer are 83 GPa at 0° (a axis) and 25 GPa at 90° (b axis). The corresponding results of $\nu$ are 1.1 and 0.3, respectively. Unfortunately, the situation of monolayer As$_2$S$_3$ is complicated where there exist two maximums for $E$ and $\nu$, separately. As for the Shear modulus $G$, similar trends can be
found for both monolayer and bilayer As$_2$S$_3$ shown in Figs. 6(c) and 6(f). The maximum $G$ is around 13 GPa for bilayer, while the minimum $G$ is 10.3 GPa and 5.9 GPa for monolayer and bilayer As$_2$S$_3$, respectively.

These results suggest that the anisotropic mechanical properties are obvious both in monolayer and bilayer As$_2$S$_3$. What is more, the outcome from the strain–energy method is also verified by Fig. 5, which confirms the correctness and consistency of our computational methods. In our present work, the anisotropic factor of monolayer and bilayer is 3.15 and 3.32, respectively, which is relatively good agreement with the previous experimental measurement [1] and is quite higher than that of BP, confirmed in experiment to be 2 [2].

Furthermore, the absolute value of Young’s modulus increases from the monolayer in Fig. 6(a) to the bilayer Fig. 6(d). Our results in $\sigma$-direction are consistent with the experimental values, but a little smaller than that of the experimental values in $\beta$-direction. This limited discrepancy is probably derived from the layer-dependent effect. In the experiment, the investigated samples are more two layers of As$_2$S$_3$, while our calculation is exactly the bilayer system [1]. However, both the experimental data and our calculated results confirm the high anisotropic mechanical properties of 2D As$_2$S$_3$ material.

We find that the highly anisotropic mechanical properties in As$_2$S$_3$ systems can be explained by $\text{As} \rightarrow \text{As}$ bond angles along $\alpha$-direction. All optimized $\text{As} \rightarrow \text{S}$ bond lengths range from 2.28 to 2.31 Å in both monolayer and bilayer As$_2$S$_3$, but they have different bond angles. We find that all the $\text{As} \rightarrow \text{S}$ bond angles can be classified into two types, one is the mainly elongated bonds along with $\alpha$-direction, called A-type shown in Figs. 1(a) and 1(b), with A-type bond angles of $89^\circ$ and $88^\circ$, respectively. In contrast, the other $\text{As} \rightarrow \text{As}$ bond angle is called B-type with a value of 102$^\circ$ and 101$^\circ$ for monolayer and bilayer As$_2$S$_3$, separately. The smaller $\text{As} \rightarrow \text{As}$ bond angle of A-type along $\alpha$-direction will enhance the strength of the $\text{As} \rightarrow \text{As}$ bonds (As$_1$ – As$_2$ in Fig. 1 and S – S bonds (S$_2$ – S$_3$ in Fig. 1(a)) along $\beta$-direction. As a consequence, large anisotropic Young’s modulus $E$ and $\sigma$ are identified and verified.

4. Conclusions

In this work, we have systematically explored the charge distribution, electronic band structures, angle-resolved effective masses, mobility, strain–stress curves, orientation-dependent Young’s modulus, Poisson’s ratio, and Shear modulus for monolayer and bilayer As$_2$S$_3$ by first-principles calculations. The result shows that monolayer and bilayer As$_2$S$_3$ have significantly large anisotropy of electronic and mechanical properties. The electronic anisotropy would make 2D As$_2$S$_3$ a superior candidate for applications in the photovoltaic field where the generated holes and electrons need to be separated. More interestingly, the calculated anisotropic factor of monolayer and bilayer As$_2$S$_3$ are 3.15 and 3.32, respectively, which are significantly higher than that of BP, showing a factor of 2. We expect our study will provide valuable guidance for orientation-related nano-devices, as well as for promoting related experimental investigations.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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