The electrical and spin properties of monolayer and bilayer Janus HfSSe under vertical electrical field

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Abstract
In this paper, the electrical and spin properties of mono- and bilayer HfSSe in the presence of a vertical electric field are studied. The density functional theory is used to investigate their properties. Fifteen different stacking orders of bilayer HfSSe are considered. The mono- and bilayer demonstrate an indirect bandgap, whereas the bandgap of bilayer can be effectively controlled by the electric field. While the bandgap of bilayer closes at large electric fields and a semiconductor to metal transition occurs, the effect of a normal electric field on the bandgap of the monolayer HfSSe is quite weak. Spin–orbit coupling causes band splitting in the valence band and Rashba spin splitting in the conduction band of both mono- and bilayer structures. The band splitting in the valence band of the bilayer is smaller than a monolayer, however, the vertical electric field increases the band splitting in bilayer one. The stacking configurations without mirror symmetry exhibit Rashba spin splitting which is enhanced with the electric field.

Keywords: Janus HfSSe, density functional theory, spin–orbit coupling, Rashba, spin-splitting, vertical electric field

(Some figures may appear in colour only in the online journal)

1. Introduction

Two-dimensional (2D) transition-metal dichalcogenides (TMDs) attract intensive attention due to their extraordinary electronic, optical, mechanical and thermal properties [1, 2]. In the layered TMDs with the chemical formula MX2 (M = Mo, W, Zr, Hf; X = S, Se, Te), the transition metal atom M is sandwiched between two chalcogen atoms X to form X–M–X configuration by strong intra-layer chemical bonding. The layers are connected with weak van der Waals forces. 2D monolayer TMDs demonstrate rich physics and potential for broad applications in the fields of electronics, optoelectronics, catalysis, and spintronics [1, 3]. TMD materials have been extensively studied due to their outstanding properties such as high carrier mobility and on/off current ratio. Most 2D TMD materials are semiconductors with a bandgap of about 2 eV which can be controlled by electric field [4, 5], making them suitable for application in nanoelectronics and optoelectronics.

The bulk HfX2 (Hafnium dichalcogenides) (X = S, Se) are TMD semiconductors with an indirect bandgap [6, 7]. These compounds with quasi-layered structures stay together with low van der Waals force. The monolayer HfS2 can be exfoliated by mechanical and chemical techniques [6, 7]. Hafnium dichalcogenides have drawn considerable attention because of its fascinating electronic and optical properties [8–10]. Particularly, these materials demonstrate high mobility (1800 to 3500 cm2Vs−1) and a large absorption range (1–2 eV). Monolayer HfS2 and HfSe2 are proposed as suitable materials for the electronic and optoelectronic applications [11–15]. These materials demonstrate potential candidate for application in next-generation nanodevices such as water splitting and large...
scale solar cell [16, 17]. Monolayer HiS$_2$ with a bandgap approximately equal to 2 eV, is theoretically confirmed to enhance the absorption portion of the sunlight for water splitting [18]. The ultra-thin HiS$_2$ with high stability is demonstrated as phototransistors with high on/off ratio, high responsivity, a small response time that shows remarkable potential for electronic and optoelectronic applications [11]. Nowadays, numerous nanodevices based on the HiS$_2$ such as photodetectors and field-effect transistors have been experimentally fabricated [12, 19–21].

Bilayer ZrSe$_2$ and HiSe$_2$ demonstrate an indirect bandgap of 0.99 and 1.07 eV, respectively [22]. These two bilayers demonstrate high hole mobility which is one order of magnitude larger than the electron. The effect of the vertical electric field on the electronic properties of bilayer ZrSe$_2$ has been investigated. The bandgap of bilayer ZrSe$_2$ decreases with rising electric field [23] and semiconductor to metal transition occurs at a critical electrical field.

Spintronics based on 2D materials has attracted increasing interest in the last decade [24]. The 2D materials with Rashba spin splitting have drawn considerable attention due to splitting tunability by an external electric field [25]. A giant Rashba spin splitting can decrease the precession time of the spin to be smaller than the spin relaxation time and is desirable for practical spintronic applications [26]. In addition to a large Rashba coefficient, Rashba spin splitting should be effectively tuned by some external conditions and experimental techniques, such as electric fields, with potential applications in spin FETs. Therefore, it is desirable to find 2D semiconductors with a large and tunable Rashba spin splitting effect. However, common TMDs are nonpolar and do not exhibit any intrinsic Rashba effect. Recently, a polar TMD monolayer, Janus MoSSe, has been successfully synthesized in experiments, in which top S atoms of MoS$_2$ are fully replaced by Se atoms [27, 28]. Due to the different electronegativity of S and Se atoms, MoSSe demonstrates an internal electric field perpendicular to the monolayer plane. Janus structures show intrinsic Rashba spin splitting induced by out-of-plane mirror symmetry breaking. Furthermore, the Rashba effect in 2D Janus TMDs can be effectively manipulated by the electric field [29]. Therefore, investigation of spin properties and Rashba effect in 2D materials is desirable and can reveal potential applications in spin FETs.

The electrical, and electronic properties of Janus ZrSSe monolayer are studied. It is confirmed that the ZrSSe monolayer has dynamically and mechanically stable. The ZrSSe monolayer is an indirect gap semiconductor and demonstrates amazing spin–orbit splitting [30]. Barhoumi et al. [31] studied the stability and electrical properties of monolayer and bilayer Janus HfSSe. The HfSSe bilayer is an indirect semiconductor, whereas, the HfSSe alternating in which the S and Se atoms are uniformly spread in the varying location, is a direct semiconductor. They studied four stacking orders of HfSSe bilayer, which display an indirect semiconductor with the bandgap in a range of 0.361–0.830 eV.

To the best of our knowledge, there is not a comprehensive study on the spin properties of different stacking orders of bilayer HfSSe. The polar 2D TMDs will surely enrich the family of the materials with the Rashba effect and improve the progress of the spin FETs. So, it is necessary to explore the spin properties and Rashba effect in these materials. In addition, an external electric field can be used to tune the spin properties of 2D materials. Therefore, we have focused on the electrical and spin properties of mono- and bilayer HfSSe where besides the Rashba effect and band splitting, we have investigated the effect of external electric field using density functional theory. Janus bilayer HfSSe with fifteen stacking orders is considered. We have found the Rashba-type spin splitting around the $M$ point of the conduction band for all stacking orders of bilayer HfSSe with mirror asymmetry that can be improved by the electric field and have the potential for application in spintronic devices.

2. Computational details

In order to investigate the properties of HfSSe, density functional calculations are performed using the SIESTA package [32]. The generalized gradient approximation with the Perdew–Burke–Ernzerhof (PBE) [33] functional is employed for the exchange–correlation term. We have adopted fully relativistic pseudopotentials and have taken into account the effect of spin–orbit coupling (SOC). The van der Waals interaction between layers in bilayer structures is treated using Grimme’s correction to the PBE functional [34] which is the same method described in our previous study [35, 36]. A Monkhorst-Pack $k$-point grid of $21 \times 21 \times 1$ is chosen for the unit-cell. The energy cutoff is set to be 50 Ry and a double-$\zeta$ plus polarization basis-set is used. The total energy is converged to better than $10^{-5}$ eV and the geometries are fully relaxed until the force on each atom is less than 0.01 eV Å$^{-1}$. A vacuum region of 30 Å is added to avoid interactions in the normal direction. In order to visualize the atomic structures, the XCRYSDen package has been used [37]. A vertical electric field has been applied to the structures. The effective masses of the electrons and holes are calculated as [38]:

$$m^* = \frac{\hbar^2}{\partial^2 E/\partial k^2},$$

where $h$ is reduced Planck constant, $E$ and $k$ are the energy and wave vector of the conduction band minimum (CBM) and the valence band maximum.

3. Results and discussion

The band structure of monolayer Janus HfSSe with and without spin–orbit coupling is depicted in figure 1. The optimized structural, electrical, and spin properties of monolayer HfSSe are summarized in table 1. The values of the lattice parameter and bandgap are calculated as 3.718 Å and 0.587 eV, respectively. The lattice parameter is close to the previously reported values and the bandgap is almost the average value of the band gaps previously reported which are in the range of 0.45 to 0.834 eV [31, 39–41]. Comparing figures 1(c) and (d) one
The structural properties of the fifteen stackings are listed in Table 1. The lattice parameters are approximately the same for all stackings and are close to the lattice parameter of the monolayer. The interlayer distance (\(d_{int}\)) is in the range of 2.8 to 3.682 Å. The distance between Hf atoms of two layers (\(d_{Hf-Hf}\)) and the vertical distance between S and Se atoms in a layer (\(d_{S-Se}\)) are also reported. AA1 stacking has the lowest binding energy regardless of the vertical configuration, indicating that the AA1 structure is the most stable stacking order. In AA3 and AB1 structures, the lowest chalcogen atom of the top layer is exactly located on the top of the highest chalcogen atom of the bottom layer (see figure 2). This results in a repulsive electrostatic interaction between these atoms and the largest interlayer distance and binding energy in these structures. Therefore, the van der Waals interaction is lower in these two structures which results in the most unstable structures. However, other structures can effectively avoid the electrostatic repulsive interaction.

**Table 1.** The structural parameters (\(a\) and \(d_{S-Se}\)), bandgap (\(E_g\)), the band splitting at \(\Gamma\) point (\(\lambda_{\Gamma}\)), Rashba coefficient (\(\alpha_R\)) and the effective masses of electron and hole in monolayer HfSSe. The length, effective mass, energy, and Rashba coefficient are in the units of Å, \(m_0\), eV, and eV Å respectively. \(m_0\) stands for the electron rest mass.

| \(a\) | \(d_{S-Se}\) | \(E_g\) | \(E_C - E_V\) | \(\lambda_{\Gamma}\) |
|-------|-------------|--------|----------------|----------------|
| 3.718 | 0.043       | 0.587  | 0.313          | 0.203          |
| \(m_{e,\Gamma}\) | \(m_{h,\Gamma}\) | \(m_{e,\Gamma}\) | \(m_{h,\Gamma}\) | \(\alpha_R\) |
| 0.212 | 0.191       | 2.116  | 0.197          | 0.159          |

can conclude that SOC splits the degeneracy of first and second bands at \(\Gamma\) point in the valence band. The value of this band splitting (\(\lambda_{\Gamma}\)) that represents the strength of spin–orbit coupling, is 0.203 eV.

HfSSe exhibits isotropic hole effective mass, whereas the electron effective mass is anisotropic. As one can see, the band structure is anisotropic around \(M\)-valley. The electron effective masses are 0.197 and 2.116 \(m_0\) along \(M-K\) and \(M-\Gamma\) paths, respectively. The first and second valence bands are close to each other at the valence band maximum (VBM). Therefore, the effective masses of first and second valence bands which are 0.212 \(m_0\) and 0.191 \(m_0\) should be considered. The electron effective masses are approximately close to HfS\(_2\) and HfSe\(_2\), whereas HfSSe demonstrates a lower hole effective mass [22, 42–46].

The minimum of the conduction band is placed at \(M\)-valley and the magnified view of the band structure around this point is depicted in figure 1(f). As one can observe, the band structure displays Rashba splitting at \(M\)-valley. Rashba coefficient can be obtained as \(\alpha_R = 2E_R/K_R\) where \(E_R\) and \(K_R\) are Rashba energy and momentum, respectively. The value of the Rashba coefficient is negligible at \(M\) to \(\Gamma\) path and we have reported it along with \(M\) to \(K\) path. The Rashba coefficient is 0.159 eV Å that is smaller than reported values for other 2D materials [29, 47–51].

In the following, bilayer HfSSe is explored and its properties are discussed. The five stacking orders are depicted in figure 2. In the vertical direction, there are three kinds of configurations for each stacking order: SeHfS/SHfSe, SeHfS/SeHfS, and SHfSe/SeHfS. We label these three vertical configurations as SS, SSe, and SeSe. Therefore, considering the three vertical configurations for each stacking order of figure 2, fifteen different stackings are obtained.

The band structures of these fifteen configurations are similar with some differences. As a sample, we consider AA1 stacking which has the lowest energy and is the most stable structure. The band structures of AA1 stacking with SS, SeSe, and SSe vertical configurations are shown in figure 3. The band structures are similar to monolayer HfSSe and exhibit an indirect bandgap. The valence band maximum and CBM are placed at \(\Gamma\) and \(M\)-points, respectively. Up- and down-spin possess the same energies in SS and SeSe stacking, whereas, spin splitting occurs in SSe configuration. Rashba property is also observed in SSe stacking and other stackings do not display any Rashba splitting.

The structural properties of the fifteen stackings are listed in Table 1. The lattice parameters are approximately the same for all stackings and are close to the lattice parameter of the monolayer. The interlayer distance (\(d_{int}\)) is in the range of 2.8 to 3.682 Å. The distance between Hf atoms of two layers (\(d_{Hf-Hf}\)) and the vertical distance between S and Se atoms in a layer (\(d_{S-Se}\)) are also reported. AA1 stacking has the lowest binding energy regardless of the vertical configuration, indicating that the AA1 structure is the most stable stacking order. In AA3 and AB1 structures, the lowest chalcogen atom of the top layer is exactly located on the top of the highest chalcogen atom of the bottom layer (see figure 2). This results in a repulsive electrostatic interaction between these atoms and the largest interlayer distance and binding energy in these structures. Therefore, the van der Waals interaction is lower in these two structures which results in the most unstable structures. However, other structures can effectively avoid the electrostatic repulsive interaction.

**Figure 1.** (a) Side and (b) top view of the atomic structure of monolayer HfSSe. The unit cell is determined with solid line. Band structure of monolayer HfSSe (c) without and (d) with SOC. The magnified view of the band structure around the (e) \(\Gamma\)-point in the valence band and (f) \(M\)-point in the conduction band.
Figure 2. (a) Side view of the atomic structures of five different stacking orders of bilayer HfSSe with SeSe vertical configuration. (b) The SS, SSe, and SeSe configurations of the AA1 stacking order. Fifteen stacking orders can be obtained by changing the position of S and Se atoms in the structures.

Figure 3. The band structure of bilayer HfSSe with configurations AA1-SS, AA1-SeSe and AA1-SSe.

tion, which is similar to the bilayer graphene and MoS2 with AB-stacking which are more stable.

The electrical and spin properties of the bilayer HfSSe are summarized in table 3. The bandgap is in the range of 0.264 to 0.426 eV that is lower than a monolayer. AA1 and AA2 stackings possess the highest and lowest bandgap, respectively. Both conduction and valence band edges are also closer to the Fermi level compared to monolayer ones. The effective masses for conduction and valence bands are listed in table 3. As one can observe, the effective masses are approximately close to monolayer where some stackings display higher and others lower values. The valence band splitting at Γ-point is in the range of 35 to 160 meV. Finally, the SSe vertical configurations display Rashba splitting due to the lack of mirror symmetry, whereas, two SS and SeSe configurations demonstrate mirror symmetry. In the following, we consider AA1 configurations due to their lower energies, whereas, similar behavior has been observed in the other stackings.

The vertical electric field is known as a useful method to tune electrical properties. The effect of vertical electric field on
the electrical and spin properties of mono- and bilayer HfSSe is explored. The interlayer distance and distance between Hf atoms of two layers as a function of the electric field are plotted in figure 4. \( d_{\text{Hf-Hf}} \) and \( d_{\text{int}} \) in SS and SSe configurations are approximately unchanged at small values of the electric field, whereas they display a decreasing behavior under larger values of the electric field. On the other hand, \( d_{\text{Hf-Hf}} \) and \( d_{\text{int}} \) in SeSe stacking demonstrates an almost monotonous decreasing pattern under the electric field.

The bandgap versus electric field in mono- and bilayer is shown in figure 5. As one can see, the effect of the electric field on the bandgap of the monolayer structure is quite weak. It slowly decreases with an increase in the electric field. On the other hand, the bandgap of bilayer decreases with the negative and positive electric field. Such behavior also reported in the bilayer ZrS\(_2\) [23]. In the presence of an external electric field, energy band edges in a semiconductor are distorted and electrons and holes are pushed toward opposite directions. As a result, the electron and hole wavefunctions become Airy functions rather than plane waves. The Airy function exhibits a tail that extends into the bandgap. This phenomenon decreases the bandgap of the semiconductor and known as the Franz–Keldysh effect. It is responsible for a tail in the absorption spectrum of semiconductors at energies below the bandgap of the materials and suggests the use of an electric field to actively tune the optical gap properties of semiconductors [52]. In 2D materials, due to the small thickness, electrons and holes pushed toward the top and bottom layers and become strongly confined, which is known as the quantum-confined Stark effect. A large bandgap tuning is achieved when a strong electric field is applied perpendicularly to the multilayer black phosphorene [53] and TMDs [54]. In monolayer TMDs with very small thickness, very low charge polarization under electric field results in a small excitonic Stark shifts of the order of a few meV [52].

### Table 2

| Stacking order | S–S | S–Se | Se–S | S–S | Se–Se |
|----------------|-----|------|------|-----|-------|
| \( d_{\text{int}} \) (Å) | 3.684 | 2.802 | 3.843 | 3.059 | 2.961 |
| \( d_{\text{Hf-Hf}} \) (Å) | 5.607 | 5.843 | 6.138 | 5.059 | 6.292 |
| \( d_{\text{S-SS}} \) (Å) | 3.046 | 3.059 | 3.058 | 2.941 | 3.064 |
| \( E_b \) (eV) | −2.958 | −2.974 | −2.974 | −2.889 | −2.931 |

ZrS\(_2\) [55], it has been reported that the influence of an external electric field on the band structure of the Janus ZrS\(_2\) is quite weak and the band structure of the Janus ZrS\(_2\) is almost unchanged in the presence of the vertical electric field. The energy gap depends linearly on the electric field with a very small change from \( E = -5 \text{ V nm}^{-1} \) to \( E = 5 \text{ V nm}^{-1} \) which is about \( \Delta E_g = 0.056 \text{ eV} \). In addition, it has been approved that in comparison with bilayer MoS\(_2\) bandgap modulation due to the vertical electric field has not been observed in monolayer MoS\(_2\) and electric fields with similar magnitude induced very small change and deformation in the band structure of monolayer MoS\(_2\) [56]. Furthermore, this effect has been observed in the other monolayer 2D materials such as InSe. Wang et al. [57] have reported that there is no significant change in the band structure of monolayer InSe under electric fields due to relatively small charge polarization. At equilibrium condition, AA1 configurations have approximately the same bandgap values, see table 2. With applying the electric field, AA1-SS stacking shows a steeper decreasing pattern compared to SeSe and SSe structures. Eventually, the bandgap of three configurations closes at a field strength of \( \pm 7 \text{ V nm}^{-1} \). So, we have plotted all figure in this range.

The effective masses and the energies of conduction and valence band edges are also investigated with the variation of the electric field. The effective masses do not show any changes and remain constant under the vertical electric field. On the other hand, the value of the CBM decreases and the VBM increases with the electric field, see figure 6. The second valence band displays a local maximum at a field strength of 0 V nm\(^{-1}\). This band decreases under small electric fields and then increases for larger fields. The second valence band maximum in SS stacking demonstrates the highest local maximum and SeSe owns the smallest. These results indicate that SS stacking possesses the highest bonding and the interlayer bonding decreases in SeSe stacking.

The energy difference between the first and second valence band edges determines the contribution of the second band on the hole properties. The Band splitting at \( \Gamma \)-point in the valence band of mono- and bilayer under various electric fields are compared in figure 7. Band splitting of the monolayer is larger than that of the bilayer and decreases smoothly with the electric field. Bilayer configurations demonstrate small \( \lambda_\Gamma \) at equilibrium condition that increases sharply at low electric fields and changes slowly at larger electric fields. In the SS and SSe structures with mirror symmetry, the variation of \( \lambda_\Gamma \) at large negative and positive electric fields is symmetric, whereas in SSe structure the \( \lambda_\Gamma \) increases smoothly at negative fields and decrease slowly at positive fields due to the lack of mirror symmetry.

Next, we have investigated the influence of the vertical electric field on the Rashba coefficient in polar HfSSe and the results are plotted in figure 8. It has been reported in table 2 that only SSe stackings demonstrate Rashba splitting. We applied the electrical field to all stackings and we found that all stackings demonstrate Rashba splitting under vertical electric field, but SSe stackings display a considerable Rashba coefficient so the Rashba coefficient is only plotted for SSe stacking. As one can observe, the Rashba coefficient variation of all stackings...
Table 3. The electrical and spin properties of the fifteen stacking orders of bilayer \( \text{HfSSe} \). The bandgap \((E_g)\), the energies of conduction \((E_c - E_F)\) and valence band edges \((E_v - E_F)\) and the band splitting at \(\Gamma\)-point in the valence band \((\lambda_\Gamma)\) are in eV unit. The effective masses at \(\Gamma\)-point for first and second valence band and at \(M\)-valley in the conduction band are in \(m_0\) unit. The Rashba coefficient at \(M\)-valley in the conduction band \((\alpha_R)\) is in eV \(\text{Å}^2\) unit.

| Stacking order | \(E_g\) | \(E_c - E_F\) | \(E_v - E_F\) | \(m^{v*}_{\Gamma,1}\) | \(m^{v*}_{\Gamma,2}\) | \(m^{c*}_{M\rightarrow K}\) | \(m^{c*}_{M\rightarrow \Gamma}\) | \(\lambda_\Gamma\) | \(\alpha_R\) |
|----------------|--------|----------------|----------------|-----------------|----------------|-----------------|----------------|-------------|----------|
| AA1 S–S       | 0.426  | −0.185         | 0.241          | 0.182           | 0.365          | 0.184           | 1.095          | 0.089       | 0        |
| S–Se          | 0.415  | −0.185         | 0.242          | 0.193           | 0.22           | 3.275           | 0.129          | 0.0925      |          |
| Se–Se         | 0.426  | −0.18           | 0.235          | 0.205           | 0.219          | 0.184           | 1.639          | 0.153       |          |
| AA2 S–S       | 0.27   | −0.148          | 0.198          | 0.182           | 0.193          | 0.184           | 1.64           | 0.067       | 0        |
| S–Se          | 0.264  | −0.113          | 0.157          | 0.172           | 0.204          | 0.184           | 3.268          | 0.149       | 0.1211    |
| Se–Se         | 0.345  | −0.106          | 0.158          | 0.193           | 0.234          | 0.184           | 3.274          | 0.129       | 0        |
| AA3 S–S       | 0.405  | −0.188          | 0.244          | 0.191           | 0.313          | 0.221           | 3.439          | 0.035       | 0        |
| S–Se          | 0.387  | −0.18           | 0.225          | 0.182           | 0.182          | 0.157           | 1.636          | 0.064       | 0.1429    |
| Se–Se         | 0.347  | −0.169          | 0.219          | 0.193           | 0.184           | 1.642          | 0.13          | 0          |          |
| AB1 S–S       | 0.376  | −0.154          | 0.206          | 0.173           | 0.183          | 0.183           | 1.645          | 0.035       | 0        |
| S–Se          | 0.292  | −0.166          | 0.21           | 0.183           | 0.194          | 0.183           | 1.645          | 0.123       | 0.0924    |
| Se–Se         | 0.36   | −0.12           | 0.173          | 0.173           | 0.194          | 0.158           | 3.29          | 0.102       | 0        |
| AB2 S–S       | 0.405  | −0.16           | 0.212          | 0.182           | 0.252          | 0.184           | 1.093          | 0.092       | 0        |
| S–Se          | 0.385  | −0.178          | 0.245          | 0.193           | 0.205           | 0.184           | 3.275          | 0.119       | 0.1457    |
| Se–Se         | 0.378  | −0.171          | 0.226          | 0.205           | 0.158           | 1.638          | 0.168         | 0          |          |

Figure 4. (a) Interlayer and (b) Hf–Hf distance of AA1 stacking of bilayer \( \text{HfSSe} \) with SS, SeSe and SSe vertical configurations as a function of electric field.

Figure 5. The band gap for mono- and bilayer \( \text{HfSSe} \) as a function of electric field. AA1-SS, AA1-SeSe and AA1-SSe stackings are considered.

Figure 6. The variation of conduction band at \(M\)-point, first and second valence bands at \(\Gamma\)-point in bilayer \( \text{HfSSe} \) with AA1-SS, AA1-SeSe and AA1-SSe stackings as a function of electric field. The parameters are close to each other, therefore, \(\alpha_R\) is not affected by stacking order. The Rashba parameter increases with increasing electric field for all stackings. Such an increasing behavior of \(\alpha_R\) with electric field is previously reported in other 2D materials [58–60]. The polar structure such as SSe stackings produces a nonzero potential gradient and internal electric field normal to the surface, which induces the Rashba spin splitting. This is due to the lack of mirror symmetry. When a positive electric field is applied, according to the principle of superposition of the field intensity, the internal electric field between S and Se is strengthened. This results in an increase in the Rashba parameter. The situation is reversed when a negative electric field is applied, and the internal electric field between S and Se, and as a result, the Rashba effect is weakened.
4. Conclusion

The electrical and spin properties of mono- and bilayer HfS\textsubscript{2}Se are studied in the presence of the vertical electrical field. In monolayer structure, the value of band splitting at \( \Gamma \)-point in the valence band is 0.203 eV, and the Rashba coefficient at \( \Delta \)-point is smaller than that of the monolayer, the electric field increases it in bilayer structures so that it reaches band splitting of monolayer under a large electric field. SSe vertical configurations display Rashba splitting in equilibrium condition which is comparable to the monolayer. However, the electrical field generates Rashba splitting in all stacking orders, but the Rashba coefficient only is considerable for SSe configurations and is enhanced with the increasing vertical electric field.

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