

Research Article

Modulation Electronic Properties of Silicane/SnSe₂ Van der Waals Heterostructures Using External Force and Electric Field

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In recent years, much interest in the study of Van der Waals heterostructures (vdWhs) has arisen. This has led to a significant amount of fundamental research being produced, from which novel optoelectronic applications have been established. By using first principles, we analyze the electronic structure of silicane/SnSe₂ vdWhs in the response to an externally applied electric field and a normal strain. The results show that the silicane/SnSe₂ vdWh acts as an indirect semiconductor when it is subjected to an applied electric field between -1 and 0.1 V/Å and becomes a metal in the 0.2 to 1 V/Å range. Significantly, the electronic band alignments of the silicane/SnSe₂ vdWhs are modified from a type-II to a type-I when a field of -0.7 V/Å is applied. Furthermore, it is determined that the silicane/SnSe₂ vdWhs appears to have a semiconductor-metal phase transition at a strain of -5% . Our results indicate that the silicane/SnSe₂ vdWhs have the potential for applications in novel high-performance optoelectronic devices.

1. Introduction

Graphene, a flat mesh of hexagonal carbon atoms, was first successfully synthesized in 2004 by Novoselov et al. [1]. This was a significant step forward in the research of materials and assisted the movement of the field from the realm of the three-dimensional (3D) scale to two dimensions (2D). Since the creation of graphene, a growing number of unique 2D materials have been predicted theoretically and later synthesized experimentally, such as silicene [2–5], silicane [6–9], phosphorene [10, 11], hexagonal boron nitride [12], transition-metal dichalcogenides [13–17] (TMDs), and monolayer SnSe₂ [18–22]. However, no single 2D material possesses all the useful properties that are required for functional application in all areas. For example, silicene has limited capabilities within switching devices because of its zero-bandgap characteristics; in contrast, a typical insulator boron nitride is useful in such an application due to its very large bandgap [23–25]. Therefore, depending on the sought application, the electronic structures of existing two-dimensional materials need to be modified for each scenario.

Fortunately, it has been found that the vertical stacking of two different two-dimensional materials can enable the formation of Van der Waals heterostructures (vdWhs), which not only overcomes the drawbacks of the individual materials, but also generates unusual properties and new phenomena due to the coupling between the layers [26–29]. This discovery has extended the possible applications of two-dimensional materials for novel next-generation optoelectronic devices.

Silicane, i.e., fully hydrogenated silicene [30], has a large bandgap and a high carrier mobility [8, 9], and it is a substance that has been extensively studied since it was first synthesized by Yamanaka et al. [31]. Restrepo et al. [32] found that the application of a strain can modify the electronic structure and increase the electron mobility in silicane. Gang et al. [33] determined that the electronic structure of silicane is tunable via the application of a uniform tensile strain and an electric field. Wang and Yu [34] discovered that the bandgap of silicane can be modulated continuously by use of an applied electric field and a biaxial tensile strain. Thus, it is clear from these studies that

an applied electronic field and a strain can adjust the electronic structures of silicane. Monolayer SnSe₂, a typical group IV–VI semiconductor that contains a bandgap of 1.38 eV, is widely used in applications such as high-speed photodetection, phase-change memory, and field-effect transistors. Gonzalez and Oleynik [21] determined that the monolayer SnSe₂ possesses an indirect bandgap. Huang et al. [35] showed that the monolayer SnSe₂ sheet has a semiconductor-metal transition when placed under strain. Hien et al. [36] found that with an increasing tensile biaxial strain the bandgap of monolayer SnSe₂ raises slightly. Xia et al. [37] discovered that phosphorene/SnSe₂ vdW heterostructures possess a type-III band alignment and provides a negative differential resistance effect. These investigations demonstrated that the electronic structures of silicane and SnSe₂ can be modified by application of an electric field and a strain and by the creation of a vdWs. However, there has been insufficient research in this field, particularly for silicane/SnSe₂ vdW heterostructures. In this work, by applying both an electric field and a biaxial tensile strain, we analyze the electronic structure of silicane/SnSe₂ vdW heterostructures via density functional theory (DFT). We verify that the applied field and the strain can modify the electronic structure of the silicane/SnSe₂ vdW heterostructure.

2. Computational Methods

The computational methods of this paper are performed using calculations based on first principles and DFT. For the crystal structure relaxation and the electronic structure calculations, the generalized gradient approximation (GGA) of the Perdew–Burke–Ernzerhof (PBE) functional [38, 39] is utilized, which is part of the SIESTA code [40, 41]. The PseudoDojo method is employed to solve the Kohn–Sham equations. In these calculations, the energy cut-off is chosen as 100 Hartree. A Brillouin zone, which is useful in crystal structure relaxation, is sampled in the K-mesh of $9 \times 9 \times 1$, while a K-mesh of $11 \times 11 \times 1$ is utilized for calculations on the energy band structure. For the relaxation, the convergence energy criteria are chosen as 10^{-4} eV, and the residual force is lower than -0.01 eV/Å. To avoid unnecessary interactions between neighboring structures, the thickness of the vacuum layer is chosen to be 20 Å. Significantly, holding the mutual positions of the two material layers together requires a long-ranged vdW interaction. Here, to account for these long-range electron correlation effects, the vdW-DF3 functional is the one chosen [42].

3. Results and Discussion

To begin, the geometries of the pristine silicane and the SnSe₂ monolayers are optimized. For the pristine silicane monolayer, the relaxed lattice constants are determined as $a = b = 3.889$ Å; these value are consistent with the values determined from theory that are found in previous work [30, 33, 34]. The optimized lattice constants for the pristine SnSe₂ monolayer are $a = b = 3.921$ Å, and again this agrees with the literature values [21, 35, 36]. These results are an indication that our methods are both acceptable and

produce reliable calculations. Next, we investigate the electronic properties of pristine silicane and the SnSe₂ monolayers. The pristine silicane monolayer band structure, which is calculated by use of the PBE functional, is shown in Figure 1(a). Here, it is observed that the conduction band minimum (CBM) and the valence band maximum (VBM) are positioned at the M point and the Γ point, respectively. This signifies that pristine silicane is an indirect bandgap semiconductor, which contains a bandgap of 2.184 eV; this is consistent with the studies of Wang and Guzmán-Verri [34, 43]. Figure 1(b) shows the band structure that is calculated using the PBE functional of pristine SnSe₂. The CBM and the VBM are found at the M point and the $\Gamma \rightarrow M$ path in the two-dimensional hexagonal Brillouin zone, respectively. This indicates that pristine SnSe₂ is also an indirect bandgap semiconductor, which has a bandgap of 0.963 eV that is similar to the value (0.85 eV) determined by Li et al. [44]. The small error can be attributed to the different software packages used for the calculations. In addition, we also observe that our results are smaller than the analogous values (2.94 eV for silicane [34]; 1.46 eV for SnSe₂ [45]) that are obtained using the HSE06 method; an explanation is the possible underestimation of the bandgap by the PBE method. The correct band structure trend, and a proper understanding of the physical mechanisms, can be predicted by the standard PBE functional. To save on computational expenses, we thus use such a procedure to execute the electronic structure calculations for the silicane/SnSe₂ vdW heterostructure for both an applied electric field and a strain.

To attain the minimum lattice mismatch value, a unit cell of SnSe₂ and monolayer silicane are used to construct the silicane/SnSe₂; the determined lattice mismatch is only $\sim 0.8\%$. Compared with previous studies [22, 46–48], the obtained lattice mismatch value is extremely small, which indicates that the silicane/SnSe₂ vdW heterostructure can be constructed with ease. To determine the most stable structure, we consider six possible heterostructure stackings that are labeled as Model-I to Model-VI and correspondingly shown in Figures 2(a)–2(f).

To determine the vdW interactions between the silicane and SnSe₂ monolayers, the interface distance between the two layers (symbolized by Δ) and the formation energy (E_f) of the silicane/SnSe₂ vdW heterostructure are determined from the following equation:

$$E_f = E_{\text{total}} - E_{\text{silicane}} - E_{\text{SnSe}_2}, \quad (1)$$

where E_{total} , E_{silicane} , and E_{SnSe_2} are the total energy of the silicane/SnSe₂ vdW heterostructure, silicane, and SnSe₂ monolayer, respectively. The values calculated for E_f and Δ are provided in Table 1. Since all the calculated values for E_f are negative, we can confirm that the six stacking configurations are energetically stable and the vdW interactions between the silicane and SnSe₂ layers do exist. On examining all the configurations, we determine that the conformation Model-I is the most stable structure since it has the lowest formation energy and the smallest interfacial distance. For this reason, we solely focus on this model in the following text.

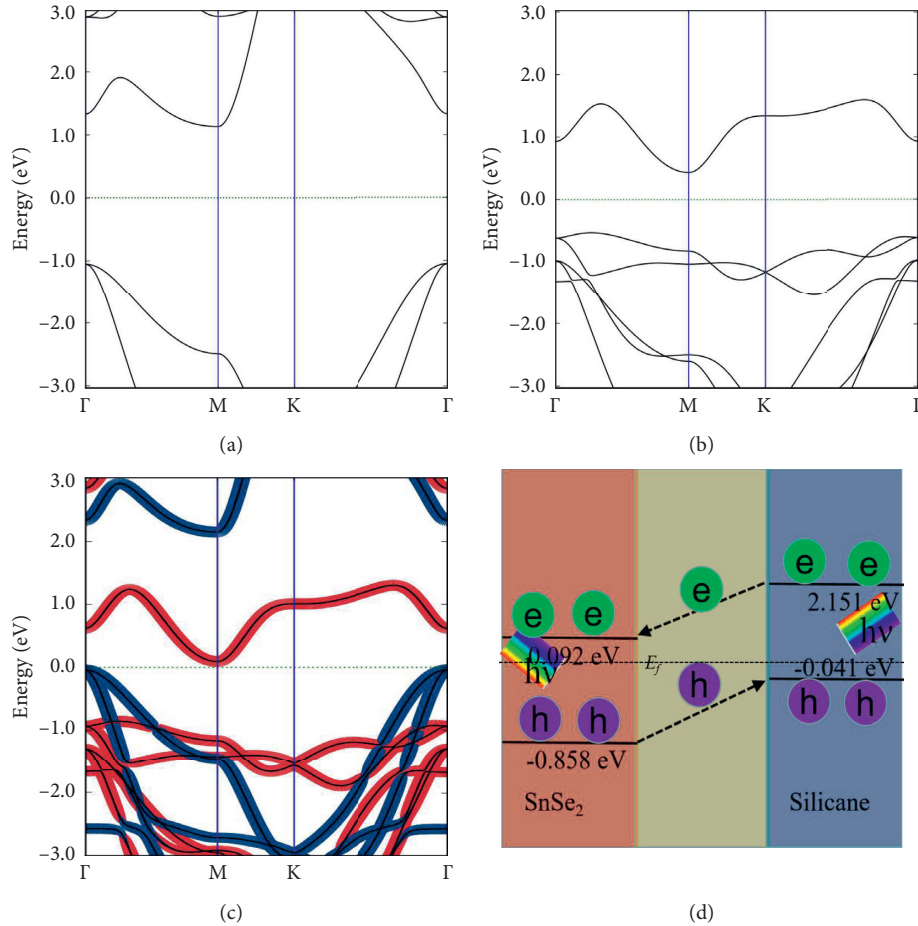


FIGURE 1: Graphs showing the band structures (in terms of units of energy) of (a) the silicane and the (b) SnSe₂ monolayers. (c) The projected band structures of the silicane/SnSe₂ vdW heterostructure are also given. Here, the dull-red lines represent SnSe₂, while the dark blue lines denote silicane. (d) A depiction of the band offset of the silicane/SnSe₂ vdW heterostructure is also provided.

Now, based on the PBE functional method, we calculate the electronic structures of the silicane/SnSe₂ vdW heterostructure (Model-I); the results are shown in Figure 1(c). The VBM predominantly derives from the silicane monolayer, and it is found at the Γ point, while the CBM principally originates from the SnSe₂ monolayer and it is positioned at the M point. From these outcomes, we can establish that the material is an indirect semiconductor that contains a bandgap value of 0.133 eV and has a type-II band alignment [49]. The bandgap of the silicane/SnSe₂ vdW heterostructure is less than those of the pristine silicane monolayer and the SnSe₂ monolayer, which indicates that the formation of the silicane/SnSe₂ vdW heterostructure can effectively modify the bandgap. To analyze the electronic structures of the silicane/SnSe₂ vdW heterostructure in greater depth, we now draw the energy band alignments of the silicane/SnSe₂ vdW heterostructures, as shown in Figure 1(d). The band edges of silicane are (2.151, -0.041) eV, while the corresponding values for SnSe₂ are (0.092, -0.858) eV. The CBM and VBM of the silicane layer are both higher than those of the SnSe₂ layer, which further confirms that the silicane/SnSe₂ vdW heterostructure has type-II characteristics [49]. These discoveries mean, due to the type-

II band alignment and the suitable bandgap value, that the silicane/SnSe₂ vdW heterostructure can be employed in high-efficiency infrared sensors.

Previous studies show that on application of an external electric field onto a vdW heterostructure system the electronic structure of the material can be substantially altered [50, 51]. Hence, under the influence of a vertical electric field, we now analyze the electronic structure of the silicane/SnSe₂ vdW heterostructure. The path of the electric field is chosen to be perpendicular to the length of the silicane/SnSe₂ vdW heterostructure: the positive direction is presumed to be from the silicane towards SnSe₂. The electric field is implemented within the range of -1.0 to 1 V/Å in steps of 0.1 V/Å. The effects of the electric field on the band edges, the bandgap, and the band structures of the silicane/SnSe₂ vdW heterostructure are illustrated in Figure 3 and Figure 1S. We determine that, in the range of -1 to 0.1 V/Å, the silicane/SnSe₂ vdW heterostructure is an indirect semiconductor, while it is a metal for 0.1 to 1 V/Å. In addition, for -1 to -0.7 V/Å, the CBM and VBM are both seen to mostly originate from the monolayer silicane, which signifies a type-I band alignment. In the range between -0.7 and 0.1 V/Å, the CBM mostly originates from the monolayer silicane, while

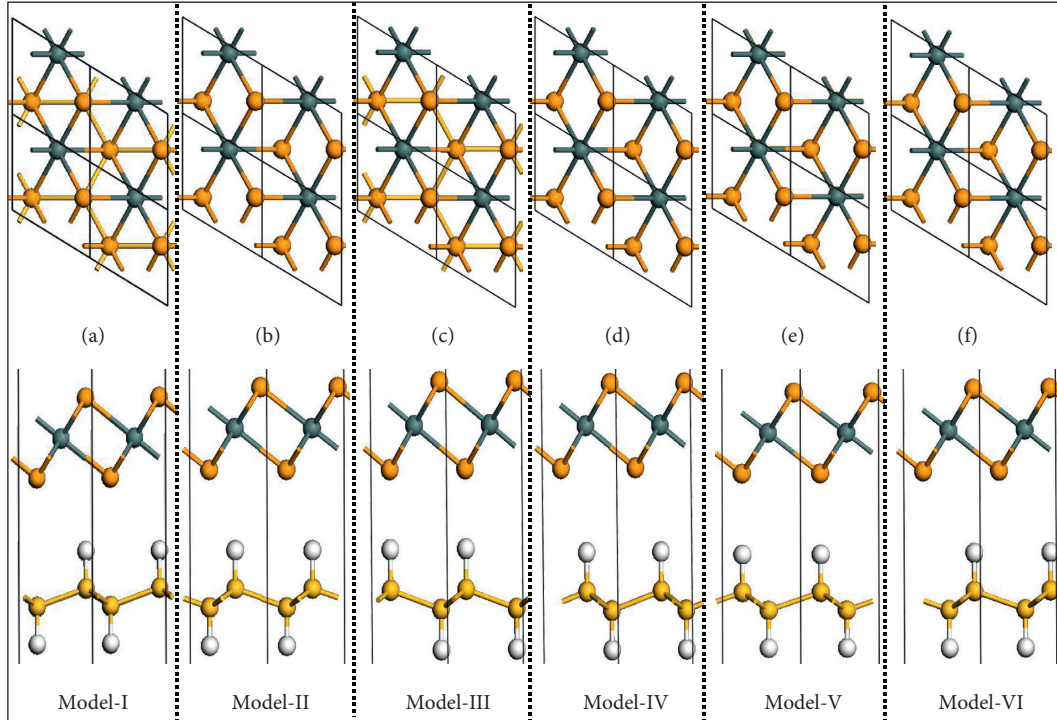


FIGURE 2: Depictions of the lattice structures (2×2) of the silicane/SnSe₂ vdW heterostructure, in which (a) Model-I, (b) Model-II, (c) Model-III, (d) Model-IV, (e) Model-V, and (f) Model-VI are illustrated. The upper diagrams show the top view, while the lower ones are the side view. The unit cells are represented by the black lines.

TABLE 1: The formation energy (E_f) of the heterostructure and the interface distance between the two layers (Δ) of the six stacking conformations.

Model	I	II	III	IV	V	VI
E_f (eV)	-0.720	-0.692	-0.688	-0.692	-0.679	-0.690
Δ (Å)	2.938	3.185	2.969	3.245	3.242	3.235

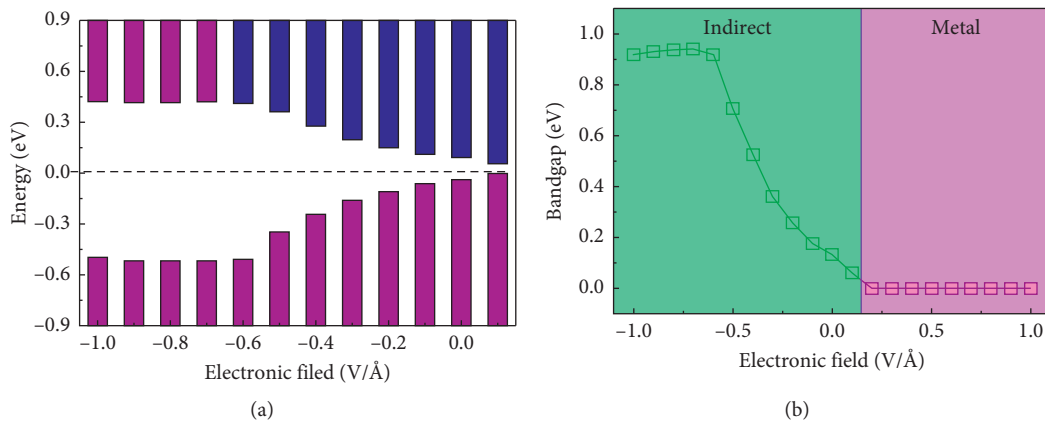


FIGURE 3: Graphs showing (a) the band edge and (b) the bandgap as a function of the external electric field strength that is applied to the silicane/SnSe₂ vdW heterostructure.

the VBM is primarily from the SnSe₂ monolayer, which suggests a type-II band alignment. These results verify that the electronic structure of the silicane/SnSe₂ vdWs is sensitive to the applied electric field.

Strain is also known as an effective regulator of the electronic structure of the vdW heterostructure [52–54]. Hence, it is now appropriate to investigate the application of an in-plane biaxial strain for the tuning of the electronic

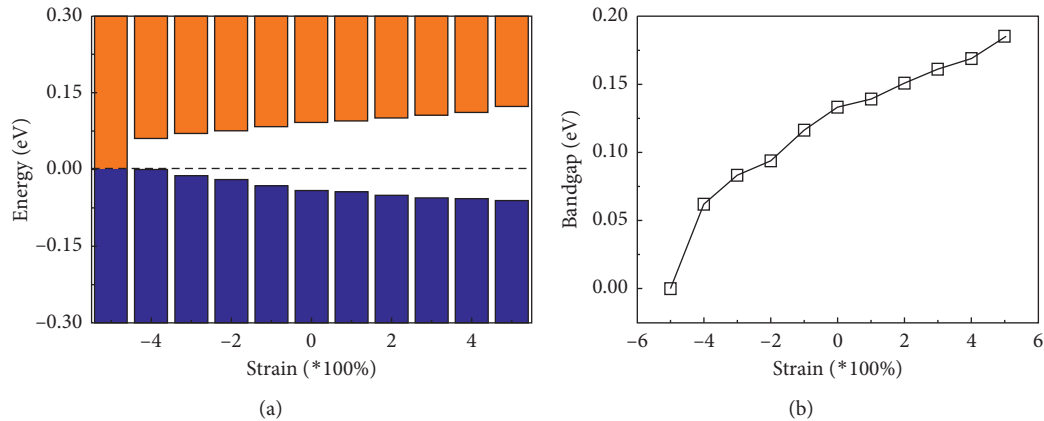


FIGURE 4: Graphs showing (a) the band edge and (b) the bandgap as a function of the strain strength that is applied to the silicene/SnSe₂ vdW heterostructure.

structure of the silicene/SnSe₂ vdW heterostructure. Such a strain is simulated by adjusting the crystal lattice parameters. They are calculated by use of the following expression:

$$\Theta = \left[\frac{(a - a_0)}{a_0} \right] \times 100, \quad (2)$$

where a_0 and a denote the unstrained and strained lattice parameters, respectively. The effects of the strain on the band edges, bandgap, and band structure of the heterostructure are shown in Figure 4 and Figure 2S. We determine that the bandgap exhibits an approximate linear increase for the strain range between -4% and 5% . Interestingly, the CBM mostly derives from the monolayer silicene, while the VBM is from the SnSe₂ monolayer, which signifies a type-II band alignment. Moreover, we found that the silicene/SnSe₂ vdW heterostructure appears to have a semiconductor-metal phase transition for a -5% strain. Therefore, effective regulation of the electronic structure of the silicene/SnSe₂ vdW heterostructure is plausible by applying a strain.

4. Conclusion

Using first principle calculations, the electronic structure of the silicene/SnSe₂ vdW heterostructure is investigated when an electric field or an in-plane biaxial strain is applied. The silicene/SnSe₂ vdW heterostructure is demonstrated to be an indirect semiconductor for cases when an electric field is implemented within the range -1 to 0.1 V/Å, while it is metallic for 0.1 to 1 V/Å. Interestingly, at an applied electric field of -0.7 V/Å, the band alignment of the silicene/SnSe₂ vdW heterostructure is modified from a type-II to a type-I. Furthermore, we determine that the silicene/SnSe₂ vdW heterostructure has a semiconductor-metal phase transition for an applied strain of -5% . The tunability of the silicene/SnSe₂ vdW heterostructure bandgap enables the possibility for practical optoelectronic device applications.

Data Availability

All data, models, and code generated or used during the study appear in the submitted article.

Conflicts of Interest

There are no conflicts of interest to declare.

Supplementary Materials

Figure 1S. Band structures of the silicene/SnSe₂ vdW heterostructure when under an applied electric field with steps of 0.1 V/Å. The upper graphs from left to right range from -1.0 to -0.1 V/Å, while the lower graphs from left to right are 0.1 to 1.0 V/Å. Here, the dull-red lines represent SnSe₂, while the dark blue lines denote silicene. Figure 2S. Band structures of the silicene/SnSe₂ vdW heterostructure when under in-plane biaxial strains with steps of 1% . From left to right, the strains range from -5% to 5% . Here, the dull-red lines represent SnSe₂, while the dark blue lines denote silicene. (Supplementary Materials)

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