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# Tunable electronic properties and related functional devices for ferroelectric $\text{In}_2\text{Se}_3/\text{MoSSe}$ van der Waals heterostructures

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In recent years, two-dimensional (2D) materials have attracted increasing attraction in a number of scientific research fields. In particular, ferroelectric materials with reversible spontaneous electric polarization and Janus transition metal dichalcogenides (TMDs) with intrinsic dipoles exhibit novel properties for many practical applications. Here, the electronic properties of van der Waals (vdW) heterostructures consisting of  $\text{In}_2\text{Se}_3$  and MoSSe were investigated based on a first-principles approach. It was demonstrated that four studied  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructures exhibited obvious band gap ( $E_g$ ) differences, ranging 0.13 to 0.90 eV for PBE (0.47 to 1.50 eV for HSE06) owing to the reversible spontaneous electric polarization of  $\text{In}_2\text{Se}_3$  and different intrinsic dipole of MoSSe, and different band alignments of type-I or type-II could also be obtained. The energy bands of the four vdW heterostructures could be obviously regulated by varying degrees of vertical (horizontal) strain and vertical interface electric field, and the  $E_g$  varied from zero to 1.27 eV. Then, M4-based mechanical switching devices and ferroelectric diodes were designed based on the significant strain and electric field function. These results provide one possible mechanism for how the polarization direction regulates the physical properties of the system due to the different charges on the two surfaces of the out-of-plane polarized ferroelectric material, which may lead to different proximity effects on the face of the material.

 Received 8th October 2022  
 Accepted 7th December 2022

DOI: 10.1039/d2ra06337a

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## 1 Introduction

Since the exploration into graphene in 2004, numerous two-dimensional (2D) materials have been reported,<sup>1,2</sup> including h-BN,<sup>3</sup> g-C<sub>3</sub>N<sub>4</sub> (ref. 4 and 5) and transition metal dichalcogenides (TMDs).<sup>6–8</sup> These 2D materials have the advantages of large surface areas and short carrier migration paths; thus, they have good photocatalytic properties.<sup>9–11</sup> Among these materials, TMDs have become one of the most interesting 2D materials in the scientific community because of their novel properties, and they have consequently been applied in many fields, such as energy storage, field effect transistors (FETs), and solar cells. The Janus MoSSe monolayer in TMDs imparts unique electronic and optical properties,<sup>12–15</sup> which emerges when the out-of-plane structural symmetry of MoS<sub>2</sub> monolayers is broken by chemical vapor deposition.<sup>16,17</sup> When one side of the MoS<sub>2</sub> monolayer has S atoms replaced by Se, the Janus MoSSe monolayer can be obtained. In terms of its electronic properties, the Janus MoSSe monolayer has built-in electric dipoles due to the broken symmetrical structure.<sup>18,19</sup> Optically, it is a material with efficient hydrogen evolution reaction (HER) activity,<sup>20</sup> but its oxygen evolution reaction (OER) activity is poor in

photocatalytic applications.<sup>21</sup> The ferroelectric material  $\text{In}_2\text{Se}_3$  is also in the spotlight with unique electronic and optical properties. It has been proved that the ultrathin  $\text{In}_2\text{Se}_3$  can form spontaneous polarization as it has a special asymmetric structure according to the existing theoretical calculations and experimental results.<sup>22,23</sup> Moreover,  $\text{In}_2\text{Se}_3$  can also act as an effective photocatalyst owing to the existence of a built-in electric field, which can separate the different charge carriers.<sup>24</sup> However, owing to the existence of a critical thickness effect, reaching a proper thin film is a long-standing challenge. van der Waals (vdW) materials provide a good opportunity for exploring two-dimensional ferroelectric properties as a single atomic layer. A common approach is to construct vdW heterostructures by stacking different 2D monolayers in a specific order, which plays a large role in the combination of various different two-dimensional materials.<sup>25–27</sup> The geometry and band structure of the single layer can be protected by the stacked monolayer formed by the extremely weak vdW interactions, on the basis of which there is an opportunity to obtain excellent physical or optical properties that are different from the previous ones.<sup>28,29</sup> For example, Wang *et al.* constructed a vdW heterostructure with two-dimensional Janus MoSSe and black phosphorus monolayers, which could significantly overcome the weak OER activity of the Janus MoSSe and the problem of the excessively fast recombination of generated carriers, thus facilitating the conditions for the spontaneous overall water splitting of black

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phosphorene/SMoSe heterostructures.<sup>30</sup> The two-dimensional GeC/GaN vdW heterostructure demonstrated excellent optical advantages with a suitable band edge position, and an absorption coefficient as high as  $10^5$ .<sup>31</sup> A heterostructure composed by blue phosphorene and ZrSSe monolayers showed a type-I band alignment with an indirect band gap ( $E_g$ ), and their band alignments could be obviously regulated by the electric field.<sup>32</sup>

In this study, we constructed four vdW heterostructures consisting of  $\text{In}_2\text{Se}_3$  and Janus MoSSe monolayers, and defined them as  $\text{In}_2\text{Se}_3/\text{SMoSe}(\text{SeMoS})$  according to the different interfaces between the two monolayers and the electric dipole direction of the  $\text{In}_2\text{Se}_3$  monolayer. The results demonstrated that these heterostructures exhibited an obvious  $E_g$  difference owing to the reversible spontaneous electric polarization of  $\text{In}_2\text{Se}_3$  and different intrinsic dipoles of MoSSe, and also that the electronic properties of the four devices could be regulated by varying the degrees of the vertical (horizontal) strain and the vertical interface electric field, thus proving the design of a mechanical switch device and ferroelectric diode based on the M4 stacking order (see Section 3.1) according to the strain and electric field function.

## 2 Models and methods

The geometry construction and calculations of the device properties were performed by density functional theory (DFT) using the Atomistix ToolKit software,<sup>33</sup> which has been widely employed in simulation studies of low-dimensional materials.<sup>34,35</sup> The residual force on each atom was less than  $0.01 \text{ eV } \text{\AA}^{-1}$  and the maximum step size was  $0.2 \text{ \AA}$  for ionic relaxation. The exchange–correlation potential was described through the Perdew–Burke–Ernzerhof (PBE) functional within the generalized gradient approximation (GGA). Because PBE does not account for van der Waals interactions,<sup>36–38</sup> we added the empirical dispersion correction DFT-D2 method described by the pairwise force field.<sup>38</sup> The temperature in the calculation was set to 300 K and the cutoff energy was 150 Ry, which was required in the numerical integration and solving of the Poisson equation. In order to assess the accuracy, we did a convergence test on the cutoff energy for the monolayer and heterostructure, and the test results showed that when the cutoff energy was greater than 150 Ry, the relative atomic energy would be less than  $0.001 \text{ eV}$ ; that is, the cutoff energy converges. The  $k$ -point grid sampling was set as  $11 \times 11 \times 1$  for norm conservation of the Troullier–Martins pseudopotential. We set a vacuum layer of length  $30 \text{ \AA}$  in the  $z$ -axis direction to avoid the effect of repeated images.

## 3 Results and discussion

### 3.1 Structure and electronic properties of the $\text{In}_2\text{Se}_3/\text{MoSSe}$ vdW heterostructures

The supercellular vdW heterostructures consisted of  $4 \times 4 \text{ In}_2\text{Se}_3$  and  $3\sqrt{3} \times 3\sqrt{3}$  MoSSe monolayers, and the lattice constants for the unit cell for  $\text{In}_2\text{Se}_3$  (MoSSe) were  $4.19$  ( $3.23 \text{ \AA}$ ).

We stacked  $\text{In}_2\text{Se}_3$  on the MoSSe monolayer vertically to construct the vdW heterostructure, and the lattice parameters of the heterostructure  $16.76 \text{ \AA}$ . There were different surface atoms of MoSSe and different electric dipole orientations of the  $\text{In}_2\text{Se}_3$  monolayer. In order to better match the  $\text{In}_2\text{Se}_3$  and SeMoS monolayers, the generalized lattice matching (GLM) method was used to balance the relationship between the mismatched strain and atomic number.<sup>39,40</sup> Four possible stacking orders of  $\text{In}_2\text{Se}_3/\text{MoSSe}$  were considered, namely M1, M2, M3, and M4. For M1 (M2), the Se (S) atoms of MoSSe faced  $\text{In}_2\text{Se}_3$ , with the electric dipole of the  $\text{In}_2\text{Se}_3$  monolayer pointing upwards, as seen in Fig. 1(a) and (b), defined as M1( $\text{In}_2\text{Se}_3/\text{SeMoS}$ ) and M2( $\text{In}_2\text{Se}_3/\text{SMoSe}$ ), respectively. For M3 (M4), the S (Se) atoms of MoSSe faced  $\text{In}_2\text{Se}_3$  with the electric dipole of  $\text{In}_2\text{Se}_3$  pointing downwards, defined as M3( $\text{SeMoS}/\text{In}_2\text{Se}_3$ ) and M4( $\text{SMoSe}/\text{In}_2\text{Se}_3$ ) in Fig. 1(c) and (d). The interlayer distances were  $3.70$ ,  $3.56$ ,  $3.64$ , and  $3.58 \text{ \AA}$  for M1–M4 with the most stable stacking structures, respectively. In the following, we calculate the binding energy of M1–M4, and the formula for the binding energy is:  $E_b = (E_{\text{HS}} - E_{\text{In}_2\text{Se}_3} - E_{\text{MoSSe}})$ , where  $E_{\text{HS}}$ ,  $E_{\text{In}_2\text{Se}_3}$ , and  $E_{\text{MoSSe}}$  represent the total energy of the heterostructure,  $\text{In}_2\text{Se}_3$ , and MoSSe monolayer, respectively. If the components of a system are separated to infinity, a certain amount of energy is required to overcome the attraction. The calculated binding energies were  $-940$ ,  $-1220$ ,  $-1310$ , and  $-1120 \text{ meV}$  for M1–M4. To gain an insight into the nature of the binding energy, based on previous studies,<sup>41,42</sup> we calculated the binding energy again using the formula:  $E_b = E_{\text{vdW}} + E_{\text{SR}}$ , where the short-range energy is  $E_{\text{SR}}$ , as described by the PBE exchange–correlation functional, and the long-range vdW attraction energy is  $E_{\text{vdW}}$ . For M1–M4, the values of  $E_{\text{SR}}$  were  $75$ ,  $108$ ,  $130$ , and  $85 \text{ meV}$ , and the  $E_{\text{vdW}}$  values were  $-1015$ ,  $-1328$ ,  $-1440$ , and  $-1205 \text{ meV}$ . These calculations prove that the formation of these heterostructures were energetically advantageous and were in agreement with the literature.<sup>41,42</sup>

We calculated the energy band structures of the isolated  $\text{In}_2\text{Se}_3$  and MoSSe monolayers with PBE (HSE06) calculations, as shown in Fig. 2(a) and (b). It could be seen that the  $\text{In}_2\text{Se}_3$  exhibited an indirect  $E_g$  with  $0.81 \text{ eV}$  ( $1.34 \text{ eV}$ ), and the conduction band minimum (CBM) was located at the  $\Gamma$ -point, while the valence band maximum (VBM) was located between the  $\Gamma$ - and  $k$ -points. For the MoSSe monolayer, both the VBM and CBM were seated at the  $\Gamma$ -points, and the value of the direct  $E_g$  was  $1.64 \text{ eV}$  ( $2.08 \text{ eV}$ ), which basically agreed with the theoretical values ( $0.81$  and  $1.54 \text{ eV}$ ).<sup>43,44</sup> The energy band structures for M1–M4 with the PBE (HSE06) calculation in Fig. 2(c) and (d), and the values of  $E_g$  were  $0.87$  ( $1.49$ ),  $0.90$  ( $1.50$ ),  $0.56$  ( $0.70$ ), and  $0.13 \text{ eV}$  ( $0.47 \text{ eV}$ ). We could see that the band structures calculated by the PBE and HSE06 were basically similar, especially for those around the Fermi level, and the band gap types were exactly the same. The PBE calculation obviously underestimated the band gap size, and thus the HSE06 calculation is generally believed to give more precise results for the band gap of a material. However, there are larger calculation difficulties if the HSE06 is used. Therefore, we only performed PBE calculations rather than HSE06 calculations to reduce the calculation

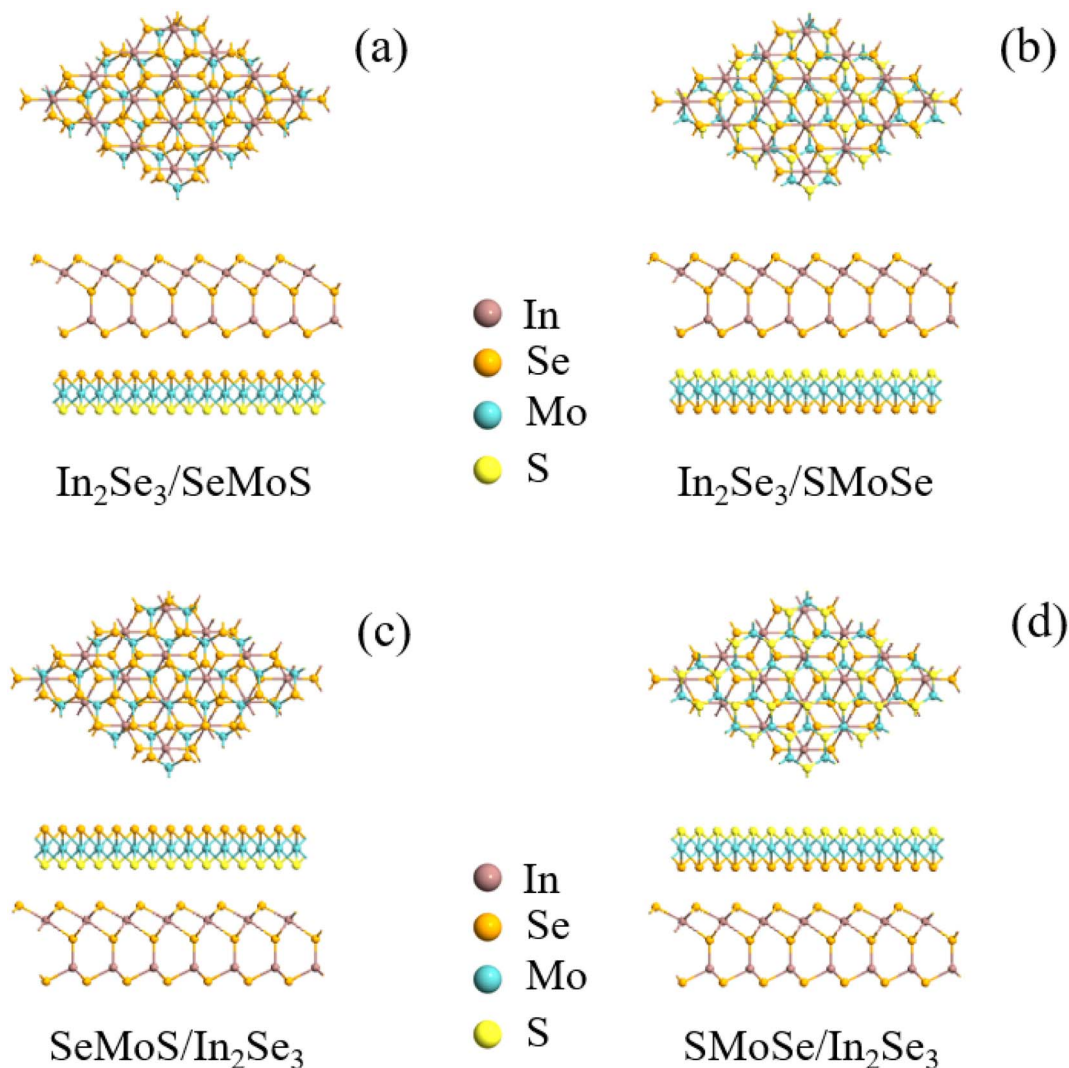


Fig. 1 Four In<sub>2</sub>Se<sub>3</sub>/MoSSe heterostructures as M1–M4: top and side views of (a) M1, (b) M2 (c) M3, (d) M4. The brown, gold, yellow, and blue represent In, Se, S, and Mo atoms, respectively.

cost for various modulations of the heterostructures and we believe that such an impact on the calculated results was acceptable.

Fig. 3 shows the projected band structures (Fig. 3(a), (c), (e) and (g)) and the projected density of states (PDOS) (Fig. (b), (d), (f) and (h)) for the four different M1–M4 systems. As shown in Fig. 3(a), M1 clearly showed a direct  $E_g$  of 0.87 eV, with both the CBM and VBM seated at the  $\Gamma$ -points. The PDOS of the M1 heterostructure indicated that the CBM originated from the In<sub>2</sub>Se<sub>3</sub> monolayer, while the VBM was contributed by the In<sub>2</sub>Se<sub>3</sub> and MoSSe monolayers in Fig. 3(b). For M2, which also showed an indirect  $E_g$  of 0.90 eV in Fig. 3(c), the CBM (VBM) was also derived from the In<sub>2</sub>Se<sub>3</sub> monolayer, which was a typical type-I band arrangement, as shown in Fig. 3(d). Therefore, two types of charge carriers tend to be transported from MoSSe to In<sub>2</sub>Se<sub>3</sub> due to the band shift, which favors recombining holes and electrons, and so type-I heterostructures have promising applications in light-emitting diodes (LEDs) and lasers.<sup>45,46</sup> For

M3, it had a direct  $E_g$  of 0.56 eV, as seen in Fig. 3(e), and CBM originated from the In<sub>2</sub>Se<sub>3</sub> monolayer, while the VBM was contributed mainly by MoSSe monolayers and a small amount by the In<sub>2</sub>Se<sub>3</sub> monolayer, as seen in Fig. 3(f). While for M4, there was a narrow direct  $E_g$  of 0.13 eV, and the VBM was further away from the Fermi level ( $E_f$ ) than the CBM. Moreover, the conduction and valence bands with a broad energy region originated from the In<sub>2</sub>Se<sub>3</sub> and MoSSe monolayers, respectively. These data indicate a typical arrangement of type-II bands. According to our previous study on the type-II band alignment,<sup>47</sup> the electrons in the MoSSe monolayer will move toward the CB of the In<sub>2</sub>Se<sub>3</sub> monolayer, while the holes in the In<sub>2</sub>Se<sub>3</sub> monolayer will shift to the VB of the MoSSe monolayer. This band alignment could effectively separate electrons and holes, and thus could be used in the field of optoelectronic devices.<sup>48,49</sup>

From the analysis of the above results, it can be seen that the In<sub>2</sub>Se<sub>3</sub>/MoSSe vdW heterostructures have the characteristics of various energy band structures, including a type-I band

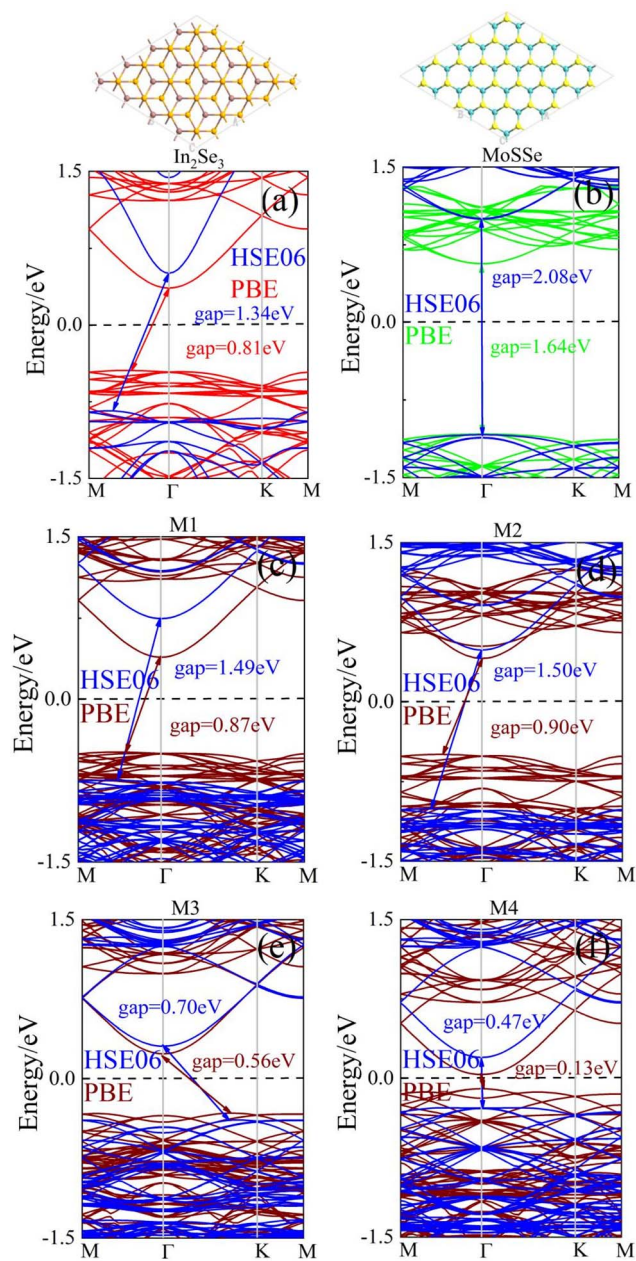


Fig. 2 Band structures for (a)  $\text{In}_2\text{Se}_3$  monolayer, (b)  $\text{MoSSe}$  monolayer, (c) M1, (d) M2, (e) M3, and (f) M4 by PBE (HSE06).

arrangement and type-II band arrangement. To better understand them, we calculated the charge density difference between M1–M4 to show the charge transfer between  $\text{In}_2\text{Se}_3$  and  $\text{MoSSe}$ , as shown in Fig. 4. It is well known that Janus  $\text{MoSSe}$  monolayers have an intrinsic layer dipole moment from Se to S atoms in the layer.<sup>50</sup> Meanwhile, the  $\text{In}_2\text{Se}_3$  monolayer also has upward or downward electric dipoles.<sup>51</sup> In addition, a weak dipole moment also existed in the interface region between the S in  $\text{MoSSe}$  and the Se atomic layers in  $\text{In}_2\text{Se}_3$ . The plane charge density difference  $\Delta\rho(Z)$  calculation formula is  $\Delta\rho(Z) = \int \rho_{\text{H}}(x, y, z) dx dy - \int \rho_{\text{In}_2\text{Se}_3}(x, y, z) dx dy - \int \rho_{\text{MoSSe}}(x, y, z) dx dy$ , where  $\rho_{\text{H}}(x, y, z)$ ,  $\rho_{\text{In}_2\text{Se}_3}(x, y, z)$ , and  $\rho_{\text{MoSSe}}(x, y, z)$  represent the charge densities of the heterostructure,  $\text{In}_2\text{Se}_3$ ,

and  $\text{MoSSe}$  at a certain point  $(x, y, z)$ , respectively. The positive ( $\Delta\rho(Z) > 0$ ) and negative values ( $\Delta\rho(Z) < 0$ ) represent electron accumulation and depletion (hole accumulation). Fig. 4 shows the corresponding isosurfaces for the difference in charge density, and it is clear that the charge was transferred from  $\text{MoSSe}$  to the  $\text{In}_2\text{Se}_3$  monolayer, but the degree of charge transfer was different for the four systems. The electrons and holes accumulate in the  $\text{In}_2\text{Se}_3$  and  $\text{MoSSe}$  region. There was more charge transfer in M2 (M3) than M1 (M4), which originated from the different interfacial effects as well as the BP/ $\text{MoSSe}$  heterostructures.<sup>50</sup>

### 3.2 Vertical strain effects on the $\text{In}_2\text{Se}_3/\text{MoSSe}$ vdW heterostructures

To explore the regulation of the interlayer distance on the electronic properties affecting the coupling interaction and electron distribution of the interface, we calculated the  $E_{\text{g}}$  changes of M1–M4 under a series of vertical strains ( $\varepsilon$ ) from  $-0.8 \text{ \AA}$  to  $+0.8 \text{ \AA}$  with a step of 2%. Here,  $\varepsilon = d - d_0$ , where  $d$  and  $d_0$  represent the compressed (stretched) and equilibrium state interlayer distances. A positive (negative)  $\varepsilon$  corresponds to stretch (compressive) strain in Fig. 5(a) and (b). The  $E_{\text{g}}$  of M1–M4 decreased monotonously when applying stretch strain, and there was a transition between a semiconductor and metal for M1 when  $\varepsilon$  was over  $0.6 \text{ \AA}$ . With the increasing compressive strain, the  $E_{\text{g}}$  of M2 (M3) showed a slight increase at first, and then gradually dropped when  $\varepsilon$  was over  $0.4 \text{ \AA}$  for M3. However, the  $E_{\text{g}}$  of M1 and M4 showed a marked increase under compressive strain, and the maximum values reached 1.27 and 0.47 eV, which were about 1.5 and 4 times that of the equilibrium  $E_{\text{g}}$ . When  $\varepsilon$  was over  $0.6 \text{ \AA}$ , the  $E_{\text{g}}$  of M4 decreased to zero. Therefore, as shown in Fig. 7(h), an M4-based mechanical switching device could be designed, in which M4 was used as the material for the central diffusion region of the device, and the two electrodes were made of graphene and the metal. When the two electrodes are properly biased, the CBM and VBM enter the bias window to achieve a narrow  $E_{\text{g}}$  and a lower potential barrier, allowing the device to be in the “On” state, resulting in a higher current flow. By applying pressure to the heterostructure, the CBM and VBM will exit the bias window, and the higher barrier keeps the device in the “Off” state with negligible current flow. Therefore, a device with a high on/off ratio ( $I_{\text{on}}/I_{\text{off}}$ ) can be obtained.<sup>52</sup> Once the heterostructure is stretched back to equilibrium, the device returns back to the “On” state.

Fig. 5(c)–(j) show the change in band edge position of M1–M4 under  $\varepsilon = \pm 0.8 \text{ \AA}$ , which is conducive to a clear understanding of the physical mechanism of  $E_{\text{g}}$  modulation. We can see that the VBM (CBM) of M1 was shifted downwards (upwards) obviously at  $-0.8 \text{ \AA}$  compared with  $0.8 \text{ \AA}$  and the equilibrium state, leading to a distinctly increased  $E_{\text{g}}$  in Fig. 5(c) and (d). For M2, it still showed a type-I band alignment at  $0.8 \text{ \AA}$  as well as the equilibrium state, and  $E_{\text{C-In}_2\text{Se}_3}$  ( $E_{\text{C-MoSSe}}$ ) was shifted upwards (downwards) at  $-0.8 \text{ \AA}$ , thus the CBM was contributed by the  $\text{MoSSe}$  monolayers. Therefore, the transition from a type-II to type-I heterostructure for M2

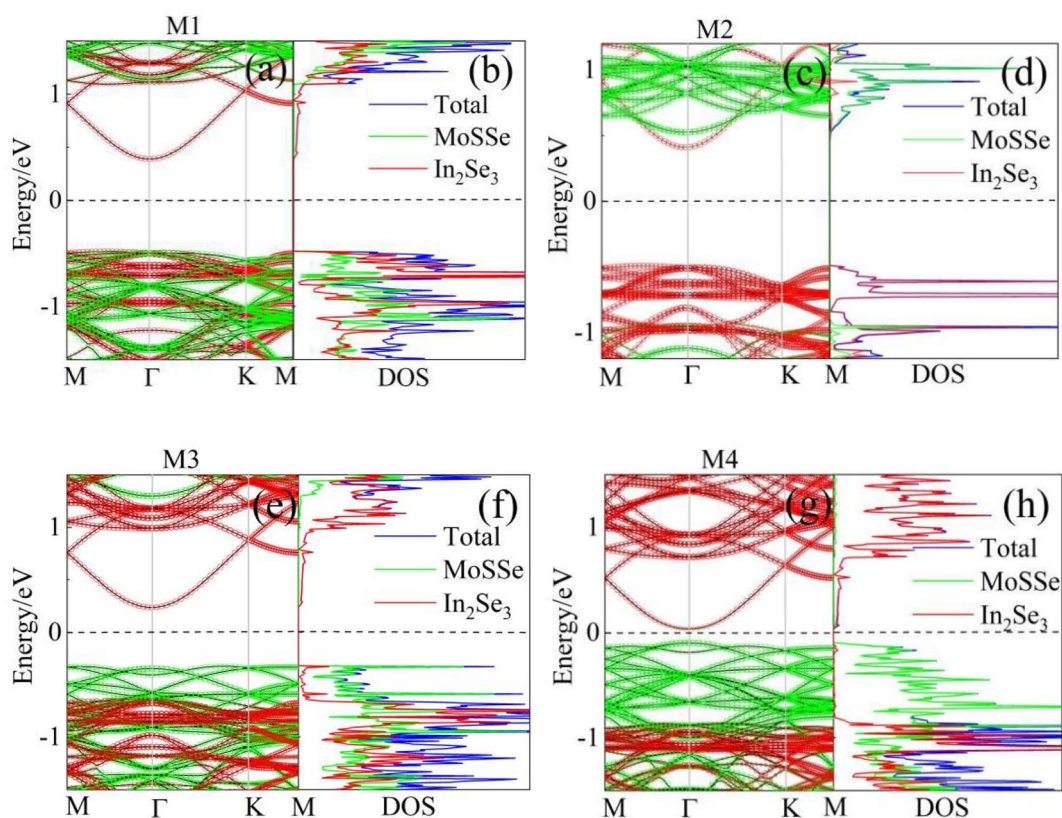


Fig. 3 Projected band structures of (a) M1, (c) M2, (e) M3, and (g) M4. Projected density of states (PDOS) of (b) M1, (d) M2, (f) M3, and (h) M4.

will be achieved with the vertical strain effect. The VBM showed a little decrease and CBM showed an opposite change compared with  $0.8 \text{ \AA}$  and the equilibrium state, and the  $E_g$  was a little augmented, as shown in Fig. 5(e) and (f). For M3, the CBM (VBM) at  $0.8 \text{ \AA}$  and  $-0.8 \text{ \AA}$  kept almost the same position, which contributed the  $\text{In}_2\text{Se}_3$  monolayer, while the VBM was contributed by the MoSSe ( $\text{In}_2\text{Se}_3$ ) monolayer at  $0.8 \text{ \AA}$  ( $-0.8 \text{ \AA}$ ), as shown in Fig. 5(g) and (h). Therefore, the  $E_g$  of M3 showed only a little change at  $-0.8 \text{ \AA}$  and  $0.8 \text{ \AA}$  strain; while the CBM contributed by the MoSSe reached the Fermi level compared with the equilibrium state for M4, and thus the  $E_g$  was zero at  $0.8 \text{ \AA}$ , as shown in Fig. 5(i), and the VBM (CBM) of M4 shifted further away from the Fermi level at  $-0.8 \text{ \AA}$ , leading to an increased  $E_g$ , as shown in Fig. 5(j).

### 3.3 Horizontal strain effects on $\text{In}_2\text{Se}_3/\text{MoSSe}$ vdW heterostructures

The horizontal stress application method is also a simple and effective method for tuning the electronic properties of a device.<sup>53</sup> Therefore, we investigated the  $E_g$  variation of M1–M4 under a range of biaxial strains ( $\epsilon$ ) from  $-8$  to  $8\%$  with a step of  $2\%$ , and  $\epsilon = (a - a_0)/a_0$ , where  $a$  and  $a_0$  are the lattice constants with and without biaxial strain. The biaxial strain was mainly applied on the basis of the vector directions  $A$  and  $B$  of the heterostructure lattice. Fig. 6(a) exhibits the schematic diagram of the  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructure by applying horizontal

stretch (positive) or compressive (negative) strain. The  $E_g$  values of the four models showed a decreasing trend under the biaxial stretch strain in Fig. 6(b), and it was noticeable that the  $E_g$  of M3(M4) reached zero when the stretch strain  $\epsilon \geq 2\%$ , and it decreased to zero under  $6\%$ – $8\%$  strain for M3. It was found that the  $E_g$  of these heterostructures increased monotonously at first, reached a maximum at  $\epsilon = 2\%$ , and then gradually decreased with the increasing compressive strain. The maximum  $E_g$  values of M1–M4 were  $1.22$ ,  $1.10$ ,  $0.65$ , and  $0.19 \text{ eV}$ , respectively. Fig. 6(c) and (d) exhibit the band structures of M1–M4 with  $6\%$  and  $-6\%$  strain. The  $6\%$  stretch strain decreased the CBM and crossed with  $E_f$  with an obvious shape change for M2–M4, while the VBM moved upwards, resulting in a transformation from a semiconductor to a metal. For M1, the CBM was still located at the  $\Gamma$ -point, but the VBM moved from the  $\Gamma$ - to the  $k$ -point, thus it converted the  $E_g$  from indirect to direct with  $\epsilon = 6\%$ . On the other hand,  $-6\%$  compressive strain made the band edge position change, but had no obvious effects on the band shape. For M4,  $6\%$  compressive strain pushed the CBM to reach the  $E_f$  and the  $E_g$  value was zero.

Fig. 6(e)–(h) show the band structures and PDOS of M1 under  $6\%$  and  $-6\%$  strain, in which we can see that the band alignment of M1 demonstrated the type-II nature with  $\epsilon = 6\%$ , and the states in the VBM comprised the  $\text{In}_2\text{Se}_3$  monolayer, but the CBM originated from the MoSSe monolayer which was different from that for the equilibrium state shown in Fig. 3(a). Moreover,

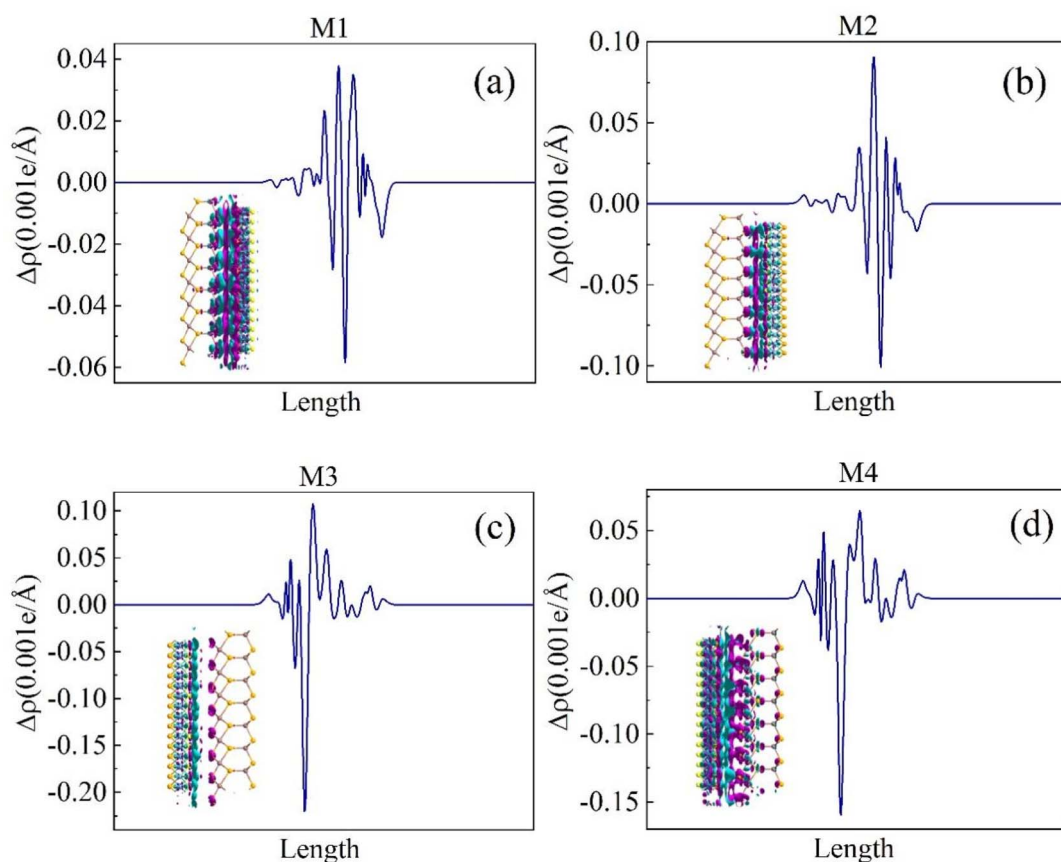


Fig. 4 Integrated charge density difference along the direction perpendicular to the interface of (a) M1, (b) M2, (c) M3, and (d) M4. Purple and cyan areas denote electron accumulation and depletion, respectively.

the CBM and VBM moved to the Fermi level, which resulted in a decrease in  $E_g$ . The conduction bands of MoSSe exhibited a down shift, while the valence bands of  $\text{In}_2\text{Se}_3$  moved up compared with the equilibrium state. When applying  $-6\%$  compressive strain, it is worth noting that the  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructure had an indirect  $E_g$  of 1.13 eV for both the CBM and VBM, showing the trend of moving away from the  $E_f$ , which was in the proper range of 1.0–1.5 eV for solar cell devices. The CBM and VBM originated from the two constituents of the heterostructure, indicating that the coupling between  $\text{In}_2\text{Se}_3$  and MoSSe was relatively strong, as shown in Fig. 6(h). As a result, the horizontal strain can greatly affect the band alignment type, the band structure shape, and the transition between a semiconductor and metal for the  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructure because the strain can induce changes in the bonds between atoms, the interfacial distances and interactions, as well as the  $\text{PC}_6/\text{WS}_2$  heterostructure.<sup>54</sup>

### 3.4 Electric field effects on $\text{In}_2\text{Se}_3/\text{MoSSe}$ vdW heterostructures

In addition, the different charge densities on the two surfaces of the out-of-plane polarized ferroelectric material can lead to different near-neighbor effects produced by the material bound to it. In conclusion, 2D ferroelectric materials with out-of-plane

polarization provide a new avenue for electric field regulation of the physical properties of stacked 2D vdW heterostructures. Tuning the external electric field ( $E_{\text{ext}}$ ) is an important way to regulate the electronic properties of these heterostructures, whereby  $E_{\text{ext}}$  is related to the vertical interface of these  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructures, as shown in Fig. 7(a), where the positive direction of  $E_{\text{ext}}$  was from the MoSSe to  $\text{In}_2\text{Se}_3$  monolayer. The electronic structure of the  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructure can vary greatly, but the geometry does not change much under different  $E_{\text{ext}}$  values.<sup>55</sup> Fig. 7(b) shows the variation of  $E_g$  with  $E_{\text{ext}}$  in the range of  $-0.6$ – $0.6 \text{ V } \text{\AA}^{-1}$  with steps of  $0.1 \text{ V } \text{\AA}^{-1}$ , where the  $E_g$  of M2 showed an obvious difference with other models under  $E_{\text{ext}}$ , whereby when a positive  $E_{\text{ext}}$  is applied to these models, the  $E_g$  of M1 (M3 and M4) decreased linearly, especially the  $E_g$  of M3, which was zero after  $E_{\text{ext}} = 0.5 \text{ V } \text{\AA}^{-1}$ . The  $E_g$  of M2 reached a maximum value of 1.05 eV with  $E_{\text{ext}} = 0.1 \text{ V } \text{\AA}^{-1}$ , and then dropped continuously with an increasing positive  $E_{\text{ext}}$ . The  $E_g$  of M2 decreased rapidly with the increasing  $E_{\text{ext}}$  under negative  $E_{\text{ext}}$ , whereby the  $E_g$  of M2 was zero after  $E_{\text{ext}} = -0.4 \text{ V } \text{\AA}^{-1}$ , and it undergoes a transition in electronic properties from a semiconductor to metal. Noticeably, when  $E_{\text{ext}} < 0$ , the  $E_g$  of M1 (M3 and M4) first linearly increased with  $E_{\text{ext}}$ , reaching a maximum value of 0.90 (1.03, 1.19) eV at  $E_{\text{ext}} = -0.1$  ( $-0.2$ ,  $-0.5$ )  $\text{V } \text{\AA}^{-1}$ . Then, it decreased gradually with

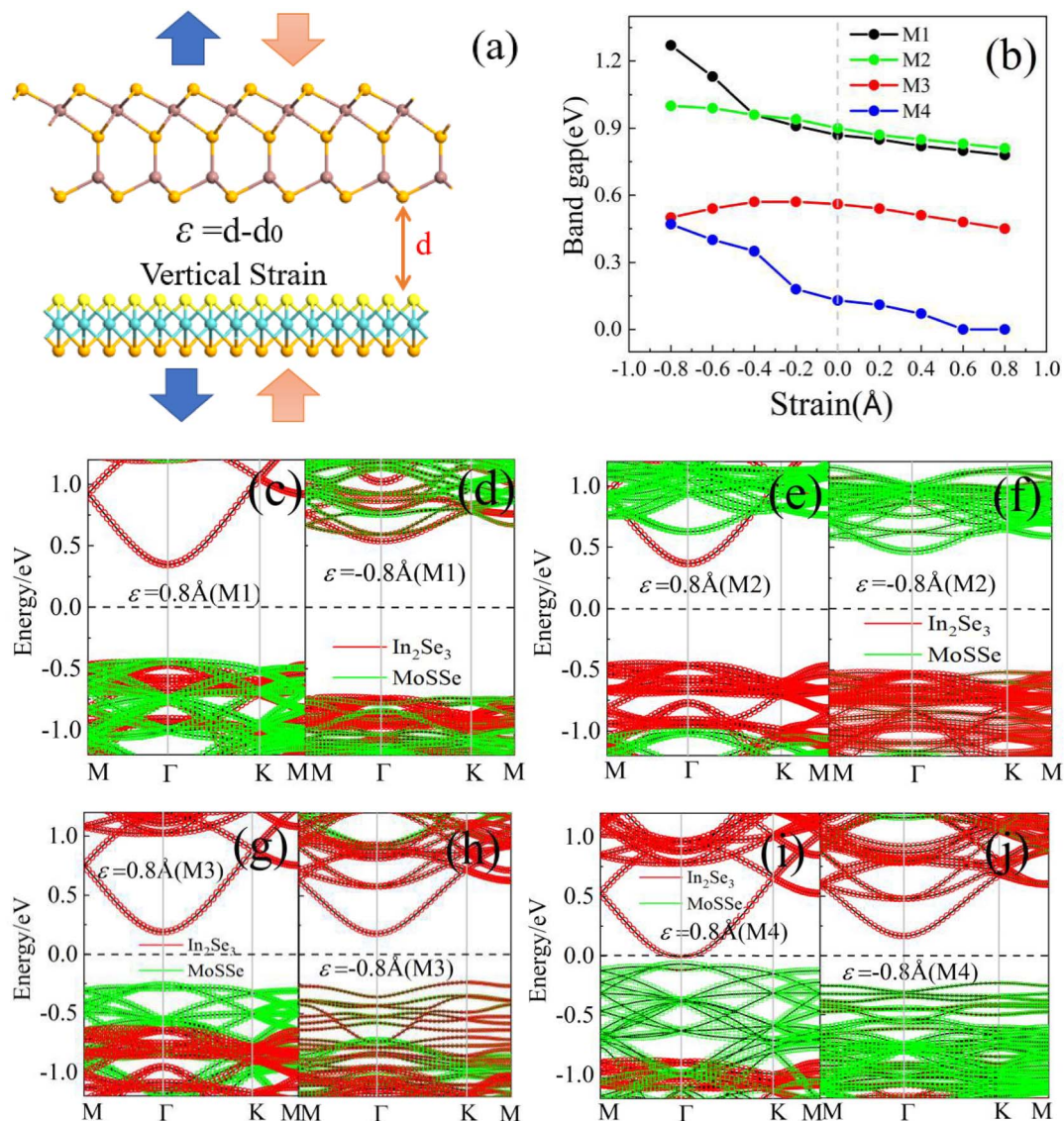


Fig. 5 (a) Schematic illustration of the synergistic effects of the vertical strain, (b)  $E_g$  as a function of the vertical strain, (c)–(j) projected band structures of the heterostructure under the selected vertical strain of  $\pm 0.8 \text{ \AA}$ .

increasing  $E_{\text{ext}}$ . Fig. 7(c) shows the variation of band structures in detail for M2 with  $E_{\text{ext}} = \pm 0.2, \pm 0.4, \text{ and } \pm 0.6 \text{ V \AA}^{-1}$ , respectively. It is clear that the band edge positions changed significantly under positive and negative  $E_{\text{ext}}$ , which fully reflected an obvious electric field effect. The DOS and PDOS of M2 at  $E_{\text{ext}} = \pm 0.2, \pm 0.4, \text{ and } \pm 0.6 \text{ V \AA}^{-1}$  are given in Fig. 7(d)–(f). For M2, it was found to belong to a type-I heterostructure at the equilibrium state, as shown in Fig. 3(c). The electric field effects led to differences in the local electrostatic potential energy (LEPE) between the  $\text{MoSSe}$  and  $\text{In}_2\text{Se}_3$  monolayers. When a positive  $E_{\text{ext}}$  acted on M2, the LEPE on the  $\text{MoSSe}$  monolayer was larger than that on the  $\text{In}_2\text{Se}_3$  monolayer, and the energy band of  $\text{MoSSe}$  ( $\text{In}_2\text{Se}_3$ ) moved monotonically upward (downward) as  $E_{\text{ext}}$  increased. We can see that the CBM states were consistently provided by  $\text{In}_2\text{Se}_3$ , but the VBM states originated by  $\text{MoSSe}$  with the applied positive  $E_{\text{ext}} =$

$0.2, 0.4, \text{ and } \pm 0.6 \text{ V \AA}^{-1}$ . This means M2 was a type-II heterostructure when  $E_{\text{ext}}$  exceeded  $0.2 \text{ V \AA}^{-1}$ . The value of the  $E_g$  of M2 depended on the CBM of  $\text{In}_2\text{Se}_3$  and the VBM of  $\text{MoSSe}$ , whereby the CBM of  $\text{In}_2\text{Se}_3$  decreased while the VBM state of  $\text{MoSSe}$  increased with the enhancement of  $E_{\text{ext}}$ , thus the value of the  $E_g$  gradually decreased. The  $E_g$  of M2 reached a maximum when the CBM states of  $\text{MoSSe}$  and  $\text{In}_2\text{Se}_3$  crossed at  $\sim 0.1 \text{ V \AA}^{-1}$ . When the electric field direction becomes a negative value, the energy band of  $\text{MoSSe}$  ( $\text{In}_2\text{Se}_3$ ) will move downward (upward), and the VBM will be provided by  $\text{In}_2\text{Se}_3$ , but the CBM states originate from  $\text{MoSSe}$ , and thus, M2 will change from a type-I to type-II heterostructure when applying a negative  $E_{\text{ext}}$ . Also, the  $E_g$  will decrease further with the CBM and VBM approaching the  $E_f$  gradually; especially, when the negative  $E_{\text{ext}}$  is over  $0.4 \text{ V \AA}^{-1}$ , the  $E_g$  will be zero for the VBM of  $\text{In}_2\text{Se}_3$  to reach or pass through the  $E_f$ . According to the above

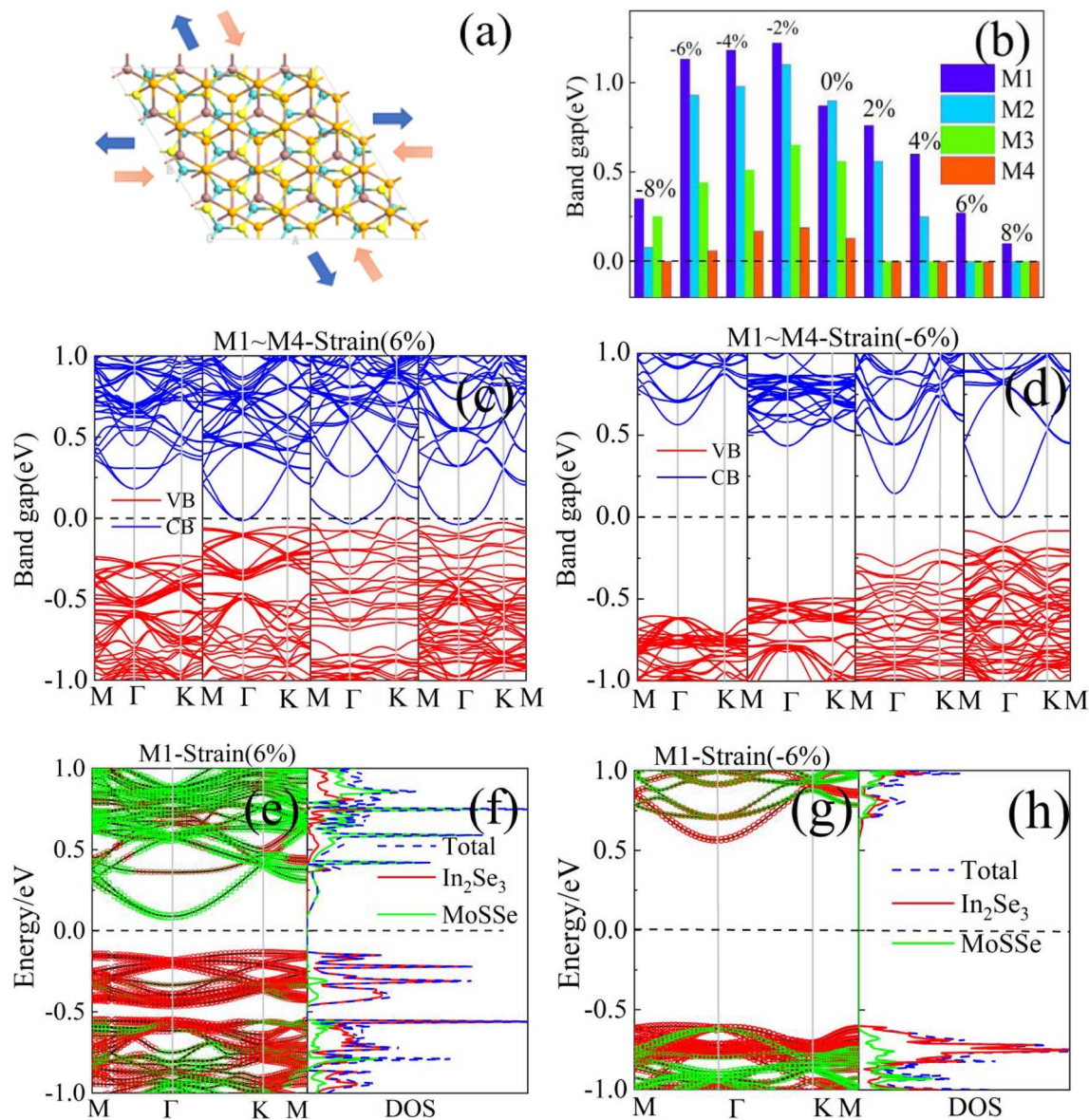


Fig. 6 (a) Schematic diagram of the In<sub>2</sub>Se<sub>3</sub>/MoSSe heterostructure under biaxial strain and (b) the  $E_g$  as a function of the horizontal biaxial strain. (c) and (d) Band structures of M1–M4 with  $-6\%$  and  $6\%$  strain, (e) and (g) the band structures, (f) and (h) the projected density of states (PDOS) under  $6\%$ , and  $-6\%$  strain for M1.

analysis process, we can also explain the various  $E_g$  values on the  $E_{\text{ext}}$  for other models. A type-II band alignment at the equilibrium state with a small  $E_g$  was observed for M4, as shown in Fig. 3(g). When a positive  $E_{\text{ext}}$  was applied, the CBM of In<sub>2</sub>Se<sub>3</sub> and the VBM of MoSSe shifted toward the  $E_f$  because of the electric field effect, resulting in the  $E_g$  diminishing rapidly at a small  $E_{\text{ext}}$ . On the contrary, the CBM of In<sub>2</sub>Se<sub>3</sub> and the VBM of MoSSe moved far away the  $E_f$ , leading to an increasing  $E_g$  under the negative  $E_{\text{ext}}$ , as shown in Fig. 7(g). For M3, the natures of the band structures were like as for M4, and the  $E_g$  showed a similar altering trend under the  $E_{\text{ext}}$ . The maximum values of  $E_g$  (0.9, 1.05, 1.03, and 1.09 eV) were obtained under different  $E_{\text{ext}}$  ( $-0.1$ ,  $0.1$ ,  $-0.2$ , and  $0.5$  eV Å<sup>-1</sup>) because of the

different moving speeds of the band edges for M1–M4. Ultimately, we briefly discuss the possibility based on the M4 heterostructure acting as a ferroelectric diode. The proposed device geometry is shown in Fig. 7(h), with the electrodes made of graphene molecular layers or metals located at each end of the heterostructured system. As can be noted from what was discussed above,  $E_{\text{ext}}$  can tune the  $E_g$  of heterogeneous structures, especially in small negative biases, where the  $E_g$  of heterogeneous structures increased dramatically in a linear form. Therefore, the transmitting current between two electrodes was very small. However, when a small positive bias was applied, the electrons could easily transit and a larger current could be obtained, showing a rectifying effect.



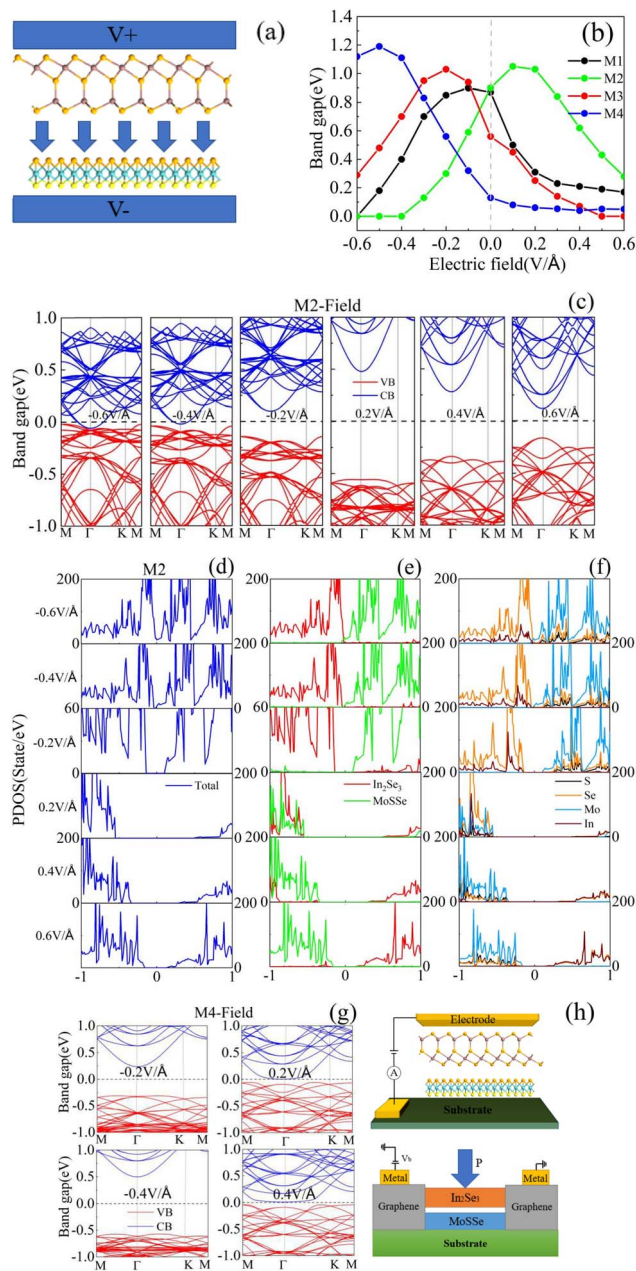


Fig. 7 (a) Schematic illustration of the synergistic effects of the external perpendicular electric field, and the positive direction of the  $E_{\text{ext}}$  from  $\text{In}_2\text{Se}_3$  to  $\text{MoSSe}$ , (b)  $E_g$  as a function of the  $E_{\text{ext}}$  for M1–M4, (c) and (g) the band structure of M2 and M4 with selected  $E_{\text{ext}}$ , (d)–(f) PDOS of M2 under the selected  $E_{\text{ext}}$  of  $\pm 0.2$ ,  $\pm 0.4$ , and  $\pm 0.6 \text{ \AA}^{-1}$ . (h) Ferroelectric diode (up) and mechanical switch device (down) based on M4.

## 4 Conclusion

In summary, the electronic properties of four  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructures were studied using density functional theory based on first-principles calculations. These results showed that these heterostructures had type-I, type-II, and other band arrangements in the intrinsic state. The four  $\text{In}_2\text{Se}_3/\text{MoSSe}$  heterostructures exhibited obvious  $E_g$  differences ranging from

0.13 to 0.90 eV by PBE (0.47 to 1.50 eV by HSE06). The energy band could be regulated effectively by the vertical (horizontal) strain, and vertical interface electric field, and then the transformation from a semiconductor to metal could be obtained. The vertical strains ( $\epsilon$ ) more obviously affected the electronic properties for M1 and M4 than for the other models. The  $E_g$  values of M1–M4 showed a decreasing trend under the biaxial stretch strain, while they increased monotonously at first, reached the maximum value at  $\epsilon = 2\%$ , and then gradually lessened with the compressive strain. The  $E_g$  variation trend of M2 was opposite to that of the other models (M1, M3, and M4) when an electric field was applied. We designed a mechanical switching device and a ferroelectric diode based on the calculated data and applied vertical strain to the model and an external electric field effect. These results demonstrated the vdW heterostructures based on reversible spontaneous electric polarization materials have more flexible regulating avenues, which could be expected to aid the design of new functional devices.

## Author contribution

Y. Zhang: investigation, formal analysis, writing the original draft. X. Q. Deng: investigation, formal analysis, conceptualization. Q. Jing: methodology, formal analysis. Z. H. Zhang: resources, supervision, project administration. X. Ding: methodology, formal analysis.

## Conflicts of interest

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

## Acknowledgements

This work was supported by Hunan Provincial Natural Science Foundation of China (Grant No. 2021JJ30733), and Hunan Provincial Innovation Foundation for Postgraduate (Grant No. CX20210828), and the Open Research Fund of Hunan Provincial Key Laboratory of Flexible Electronic Materials Genome Engineering (Grant No. 202008 and 202013).

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