Tunable reverse rectification of layed Janus MSeS (M = Hf, Zr) and SnS2 heterojunctions

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Abstract
Two-dimensional (2D) Janus transition metal dichalcogenides (JTMDs) exhibit suitable band gaps and strong visible light absorption, which are extensively applied to the field of optoelectronic devices. Here, we investigate the electronic properties of 2D JTMDs MSeS (M = Hf, Zr) and SnS2 van der Waals heterojunction through density functional theory. The calculated electronic properties reveal that ZrSeS/SnS2 heterojunction has a type-I band alignment, while HfSeS/SnS2 heterojunction has a type-II band alignment. We build the diodes based on the MSeS (M = Hf, Zr)/SnS2 heterojunctions and study the electronic transport. The currents of the devices exhibit asymmetry, and the negative turn-on voltages suggest that constructed devices are backward diodes. Moreover, it is found that the gate voltage can modulate the rectifying ratio, and the rectifying performance of ZrSeS/SnS2 is better than that of HfSeS/SnS2.

Keywords 2D JTMDs materials · Van der Waals heterojunction · Gate voltage · Backward diode · Reverse rectification

1 Introduction
The successful separation of atomic layers of single-layer graphite materials (graphene) [1] has attracted intensive research in the field of two-dimensional (2D) materials. Therefore, many researchers began to study new two-dimensional semiconductor materials, such as carbon nitride [2, 3], boron nitride [4, 5], black phosphorus [6–8], transition metal dichalcogenides materials (TMDs) [9–11] and the III–V compounds [12, 13]. Moreover, through vertically stacking different 2D materials together to form van der Waals (vdW) heterojunctions [14], it is possible to integrate the properties of a single layer while creating properties that are superior to those of single-layer material. The rich physical properties and ultra-thin thickness of 2D materials are conducive to high-density integration of devices in the vertical direction, and are easier to control than three-dimensional bulk materials, enabling further reduction in device size. Therefore, 2D heterojunctions have been recently investigated for different device applications such as transistors [15, 16], photodetectors [17, 18], photovoltaics [19, 20], and excitonic solar cells (XSCs) [21, 22].

The most ubiquitous and fundamental p-n diodes are essential building blocks of electronics and optoelectronic devices. After the advent of atomically thin van der Waals 2D materials, numerous heterostructure-based diodes have been fabricated. In fact, several high-performance diodes have been demonstrated. And TMDs have been widely used in 2D vdW heterojunction diodes. For example, vdW heterojunction photodiodes composed of BP and PdSe2 exhibit ultra-high-tunable rectification and photoresponsivity [23]. Recently, a MoTe2/ReS2 heterojunction diode has been reported, and the feasibility of constructing a photodetector has been examined [24]. The gate-tunable WSe2/SnSe2 backward diode has an impressive rectification ratio [25], etc. Nevertheless, there has not been much research on new material Janus TMDs (JTMDs) heterojunction diodes.

TMDs are considered to be very promising channel materials due to their thin atomic thickness, absence of dangling bonds, and good gate control capability [26]. However, in recent years, the novel Janus TMDs with asymmetric structure has attracted extensive attention due to their unique properties for important applications in energy conversion
technology, quantum science, and spintronics, becoming an interesting class of 2D semiconductors [27]. Due to the layered structure and narrow atomic layer thickness of 2D Janus TMDs, the 2D Janus TMDs have good tunability of electrical and optical properties and excellent mechanical flexibility. Moreover, the difference in electronegativity of sulfur-group elements, ML Janus TMDs possess an intrinsic built-in electric field, which can induce the separation of carriers [28]. Therefore, the material system has applications in microelectronics, optoelectronics, and energy devices. And there are relatively many researches on MoSeS or WSeS [29, 30], so this paper selects MSeS (M = Hf, Zr) for research. Through the chemical decomposition method, a new material called Janus TMDs (JTMDs) was synthesized experimentally [31, 32], in which a layer of sulfur in MoS2 was completely replaced by selenium. Similar JTMDs have been proven to exhibit suitable band gaps and strong light absorption from the ultraviolet to the visible light regions [33]. The experimental synthesis of MoSeS opened up a new direction for the study of layered materials. In this work, several other layered Janus transition metals dichalcogenides, HfSeS and ZrSeS are studied [34, 35]. HfSeS and ZrSeS monolayers have an indirect band gap and an ideal band gap for absorbing sunlight, which makes them suitable for electronic and optoelectronic devices. Currently, tin-based transition metal dichalcogenides (SnS2) have attracted extensive research interest due to their environmental friendliness, low cost, excellent chemical stability, semiconducting properties, high carrier mobility, and tunable electronic properties [36]. In this work, study the electronic properties and transport of MSeS (M = Hf, Zr)/SnS2 van der Waals (vdW) heterojunctions using first-principles calculations. The calculations show that the designed heterojunctions are backward diodes with an extremely high reverse rectification ratio. Moreover, we find that the gate voltage can effectively modulate the rectifying performance of the heterojunctions.

2 Model and computational details

The primitive cells of the monolayer (ML) Janus TMDs structures MSeS (M = Hf, Zr) and SnS2 are hexagonal. The rectangle unit cells of ML structures are constructed to minimize the lattice mismatch in Fig. 1a. The lattice constants for HfSSe, ZrSSe and SnS2 are b = 6.43 Å, 6.49 Å, 6.42 Å, c = 3.71 Å, 3.75 Å, 3.72 Å, respectively. The heterojunctions consisted of a 1 × 1 rectangle cell of Janus MSeS (M = Hf, Zr) and SnS2 in Fig. 1b. We construct HfSeS/SnS2 and ZrSeS/SnS2 heterojunctions, whose lattice mismatch rates are 1.36% and 2%, respectively.

All structural relaxation and calculations in this work are carried out by using the density functional theory (DFT) and non-equilibrium Green’s function method (NEGF) in the QuantumATK [37]. We use the generalized gradient approximation (GGA) [38, 39] of Perdew–Burke–Ernzerhof (PBE) [40] to describe the exchange–correlation potential. The vdW interaction is corrected with the Grimme DFT-D3 functional. The density mesh cut-off is set to 105 Hartree and the electron temperature 300 K. The k points used in the optimization of the structure and the calculations of the electronic transport properties were: 1 × 15 × 15, 5 × 1 × 150, respectively. The heterojunctions are relaxed until the forces of all atoms are less than 0.05 eV/Å. In order to avoid the interaction between adjacent layers, enough vacuum (25 Å) is added in the out-of-plane directions.

3 Results and discussion

We calculate the band structures of the pristine HfSeS, ZrSeS and SnS2 monolayers through DFT. The calculated band gaps of the monolayer HfSeS, ZrSeS and SnS2 are 0.80 eV, 0.76 eV and 1.56 eV, respectively, which agree with

![Fig. 1](image-url)  
**Fig. 1** a Rectangular unit cell of Hf/ZrSeS and SnS2, b The MSeS (M = Hf, Zr)/SnS2 heterojunction
the previous reports [41–43]. The binding energies \( E_b \) of the heterojunctions are calculated by

\[
E_b = \frac{E_{\text{MSSe/SnS}_2} - E_{\text{MSSe}} - E_{\text{SnS}_2}}{N}
\]

where \( E_{\text{MSSe/SnS}_2} \), \( E_{\text{MSSe}} \) and \( E_{\text{SnS}_2} \) are the energies of the heterojunctions and isolated monolayers, respectively, and \( N \) is the total number of atoms in the heterojunctions. The calculated binding energies of the HfSeS/SnS\(_2\) and ZrSeS/SnS\(_2\) heterojunctions are \(-0.224\) eV/atoms and \(-0.206\) eV/atoms, respectively. The negative binding energies indicate that both heterojunctions are energetically feasible.

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Then, we calculate the corresponding projected density of states (PDOS) of MSeS (\( M = \text{Hf, Zr} \))/SnS\(_2\) heterojunctions, as shown in Fig. 3. One can see that the VBM of the HfSeS/SnS\(_2\) heterojunction is mainly dominated by the Se-p orbital of HfSeS, and the CBM is mainly dominated by Sn-s and S-p orbitals of SnS\(_2\). It indicates the characteristic of a well-defined type-II semiconductor. However, the VBM and CBM of the ZrSeS/SnS\(_2\) heterojunction are both determined by ZrSeS, indicating a type-I band alignment. This result agrees with the projected energy bands in Fig. 2.

The device model is shown in Fig. 4a, the MSeS (\( M = \text{Hf, Zr} \)) region electrode is p doping, the SnS\(_2\) region electrode...
is n doping, and the doping concentration is $5 \times 10^{18}$. We study the dependence of the current $I_{ds}$ on the voltage $V_{ds}$ ($I_{ds}$–$V_{ds}$ curve) of the devices based on MSeS ($M = Hf, Zr$)/SnS$_2$ in Fig. 4. It can be seen that the $I_{ds}$–$V_{ds}$ of devices displays asymmetry. The current is almost zero in the bias voltage $-0.5$–$1$ V, while $I_{ds}$–$V_{ds}$ exhibits the linear scale at the bias voltage of $-1$–$-0.5$ V. The negative turn-on voltages suggest that constructed devices are backward diodes. In addition, the current of ZrSeS/SnS$_2$ is larger than HfSeS/SnS$_2$ at the negative bias. Thus, the rectifying performance of device ZrSeS/SnS$_2$ is better than HfSeS/SnS$_2$. The negative turn-on voltage is the same when the bias interval is $0.1$ V. But due to the different band gaps of the HfSeS/SnS$_2$ and ZrSeS/SnS$_2$ heterojunctions, the negative turn-on voltages of the two devices may be different. Therefore, we recalculate the $I_{ds}$–$V_{ds}$ curve in the negative turn-on voltage range by reducing the point interval from 0.1 to 0.05 V, as shown in the inset of Fig. 4b. The results show that the ZrSeS/SnS$_2$ device with a small band gap firstly reaches the negative turn-on voltage, which is about $-0.45$ V. And the negative turn-on voltage of the HfSeS/SnS$_2$ device is about $-0.5$ V. And since the heterojunction band gaps are very small, the difference of negative turn-on voltage is not very obvious.

The tunneling processes of the backward diode are illustrated through the band alignment in Fig. 5. Owing to the $p$ doping of MSeS ($M = Hf, Zr$) and the $n$ doping of SnS$_2$, the band edge of MSeS ($M = Hf, Zr$) shifts upward and the band edge of SnS$_2$ shifts down, as a result, an accumulation junction is formed. Under the unbiased case, the Fermi level is close to the band edge as shown in Fig. 5a. When a small negative bias is applied, electrons flow from the VBM of MSeS ($M = Hf, Zr$) to the CBM of SnS$_2$ via the band-to-band tunneling (BTBT) as shown in Fig. 5b. As the negative bias voltage increases in Fig. 5c, the energy band of MSeS rises further, while that of SnS$_2$ falls, resulting in a larger tunneling window and ultimately a larger reverse current. Under the positive bias in Fig. 5d, the tunneling window will vanish owing to the decline of the energy band of MSeS ($M = Hf, Zr$) and the rise of SnS$_2$. At the same time, the band bending also limits the carrier migration. Therefore, at the positive bias, the forward current is very small.

We calculate the transmission spectra to study the electronic transport of the devices in Fig. 6. It is known that the current depends on the integral area of the transmission spectra within the bias window. It is clear that the integral areas of both devices at $-0.8$ V are larger than those at $0.8$ V. This causes the large currents of the devices.
at −0.8 V. Moreover, compared with HfSeS/SnS2, the large integral area of ZrSeS/SnS2 at −0.8 V results in a larger current, as shown in Fig. 6b.

We further analyze the electronic transport by calculating the transmission eigenstates at ±0.8 V in Fig. 7. One can see that the devices HfSeS/SnS2 and ZrSeS/SnS2 exhibit the localization at 0.8 V, compared with the devices at −0.8 V. Thus, the currents of devices at 0.8 V are larger than those at −0.8 V, accounting for the reverse rectification. Furthermore, it is notable that there are more transmission eigenstates for ZrSeS/SnS2 at −0.8 V than HfSeS/SnS2 at −0.8 V. Consequently, the current of ZrSeS/SnS2 at the negative bias is larger than HfSeS/SnS2 as shown in Fig. 4b.

The $I_{d_{s}}-V_{d_{s}}$ characteristics of the devices at different gate voltages are shown in Fig. 8. It is clearly found that the gate voltage can effectively modulate the currents of both devices at the negative bias. But the currents hardly change at the positive bias. Thus, the gate voltage does not change the characteristics of reverse rectification of both devices. Moreover, the negative gate voltage causes a significant variation of current compared with the positive gate voltage; thus, negative gate voltage can improve rectifying performance.

The reverse rectifying ratio ($R(V) = |I(-V)_{d_{s}}|/|I(V)_{d_{s}}|$) is plotted as a function of gate voltage and $|V_{d_{s}}|$ in Fig. 9. It can be seen that the gate voltage can modulate the rectifying ratio. The device ZrSeS/SnS2 has better rectifying performance than the device HfSeS/SnS2. Notably, the rectifying ratios at negative gate voltage are larger than at positive gate voltage for both devices, which is consistent with the characteristics of the $I_{d_{s}}-V_{d_{s}}$. The rectifying ratio of the device can reach an order of magnitude of $10^7$. The reverse rectification ratio of our device is several order magnitudes higher than conventional backward diodes based on bulk materials and vdW heterojunctions backward diodes based on other 2D materials as shown in Fig. 9c. Thus, the gate voltage can modulate the rectifying performance of the device.

At $-0.8$ V. Moreover, compared with HfSeS/SnS2, the large integral area of ZrSeS/SnS2 at $-0.8$ V results in a larger current, as shown in Fig. 6b.

We further analyze the electronic transport by calculating the transmission eigenstates at $\pm 0.8$ V in Fig. 7. One can see that the devices HfSeS/SnS2 and ZrSeS/SnS2 exhibit the localization at $0.8$ V, compared with the devices at $-0.8$ V. Thus, the currents of devices at $0.8$ V are larger than those at $-0.8$ V, accounting for the reverse rectification. Furthermore, it is notable that there are more transmission eigenstates for ZrSeS/SnS2 at $-0.8$ V than HfSeS/SnS2 at $-0.8$ V. Consequently, the current of ZrSeS/SnS2 at the negative bias is larger than HfSeS/SnS2 as shown in Fig. 4b.

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Further illustrating the effect of gate voltage on electronic transport, we plot the transmission eigenstates for the present devices at the bias of $-0.8$ V at the gate voltage of $\pm 0.5$ V in Fig. 10. Both devices exhibit more eigenstates at $-0.5$ V than at $0.5$ V. The reduction in the eigenstates leads to the reduced current at positive gate voltage, as shown in Fig. 8. In addition, the device ZrSeS/SnS$_2$ has more eigenstates than HfSeS/SnS$_2$ at the gate voltage of $-0.5$ V, consequently the current of ZrSeS/SnS$_2$ is larger than HfSeS/SnS$_2$. As a result, the negative gate voltage induces better electron transmission than the positive gate voltage, which induces larger rectifying ratios at the negative gate voltage.

### 4 Conclusions

In summary, we have studied the electronic properties and transport of the MSeS ($M =$ Hf, Zr)/SnS$_2$ heterojunctions by first-principles calculations. The ZrSeS/SnS$_2$ heterojunction shows the type-I band alignment, while HfSeS/SnS$_2$ displays the type-II band alignment. The $I_{ds}$–$V_{ds}$ curves of the MSeS ($M =$ Hf, Zr)/SnS$_2$ heterojunctions display the rectifying behaviors. The larger currents of both devices at negative gate voltage than at positive gate voltage indicate that the constructed heterojunction
devices are backward diodes. The rectifying performance of ZrSeS/SnS$_2$ is better than that of HfSeS/SnS$_2$. Furthermore, the negative gate voltage can significantly change the currents of the devices, especially for ZrSeS/SnS$_2$, and improve the rectifying performance of the device. The rectifying ratio can reach up to $10^7$. The results will provide

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**Fig. 9** a and b reverse rectifying ratio of the two devices as a function of bias and gate voltage. c Comparison of rectification ratio of different backward diodes made of conventional bulk materials Si [44], GaAs [45], GaN [46], and 2D heterojunctions WSe$_2$/MoS$_2$[47], AsP/InSe [48], WSe$_2$/SnSe$_2$[25], BP/MoS$_2$[49], SnS$_2$/SiO$_2$[50]

**Fig. 10** Transmission eigenstates for the devices at the gate voltage of $\pm 0.5$ V
a guide for the high-performance rectifying device in the further.

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Declarations

Competing interests The authors have not disclosed any competing interests.

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