Research Article

Strain-Mediated Stability of Structures and Electronic Properties of ReS_2 , Janus ReSSe , and ReSe_2 Monolayers

Jia-Qi Zong, Shu-Feng Zhang, Wei-Xiao Ji, Chang-Wen Zhang, Ping Li, and Pei-Ji Wang

School of Physics, University of Jinan, Jinan, Shandong 250022, China

Correspondence should be addressed to Pei-Ji Wang; ss_wangpj@ujn.edu.cn

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Monolayers of transition metal ReX_2 and ReSX ($X=\text{S}, \text{Se}$) have been proposed as new electronic materials for nanoscale devices. In this paper, there are three structures: ReS_2 , Janus ReSSe , and ReSe_2 . Based on the first-principles theory, we analyzed the structures, electronic properties, and Fermi speed. Remarkably, we studied the stability of structures of ReS_2 , Janus ReSSe , and ReSe_2 monolayers under biaxial tensile and compressive strain by density functional approach. It is worth noting that when the strain changes, not only the band gap changes but also the band gap properties (direct and indirect) also change. The band gaps decrease with the increase of tensile strain and compressive strain; Moreover, when the strain is greater than 0, the bond angle decreases as the strain increases, and when the strain is less than 0, the bond angle increases as the strain increases.

1. Introduction

It has been proposed that the transition metal dichalcogenide (TMD) [1] ReX_2 is expected to become the next generation of new electronic materials due to the inherent electron bandgap. This led to studies on the physical and chemical properties of such structures, such as ReS_2 , ReSe_2 , WS_2 , WSSe , and WSe_2 [2, 3]. It is known from previous studies that by controlling the d-state electron of transition metal, the regulation of the band gap can be realized to make the material transition from semiconductor to semimetal or metal. More interestingly, there are also different combinations of sulfur elements [4, 5].

In multilayer 2D materials, physical properties can be regulated by external electrical/magnetic field, stress, structural modification, and heterostructure [6], which can be used to design the required optical and electronic properties of 2D materials [7]. Moreover, the effect of external electric field on a single-layer structure is not significant, such as ReS_2 , but more sensitive to a multilayer structure [8]. The heterostructure was also constructed to study 2D electron gas and interfacial superconductivity [9, 10]. Monolayer and multilayer rhenium disulfide were prepared by a mechanical cleavage method [11], and these samples were characterized.

In this way, the properties of rhenium bisulfide can be further explored and the application of rhenium bisulfide in various aspects can be better understood. Based on single layer and multiple layers of rhenium disulfide, high-performance fet is also produced. Moreover, the high-performance fet is particularly perfect in some parameters. At the same time, using the anisotropy of rhenium disulfide as the design parameter of the new device, the logical inverter was successfully prepared, and its amplification gain was also very high, so the application of rhenium disulfide in the direction of electronic device was realized [12].

When studying the electronic and optical properties of materials, the regulation of biaxial strain is more practical than that of external E-field [13]. For example, strain regulation on TMD can induce semiconductor-metal transition [14]. After such electronic regulation, it can be understood as the band gap change, and thus, carrier mobility will also change [15].

At present, there is great interest in a ReX_2 TMD monolayer system. One sulfur element, X, is replaced by another sulfur element, Y, which forms a single layer of ReXY , which is called the Janus layer and this paper is called the Janus structure [16]. One sulfur element replaces another sulfur element to provide another degree of freedom in the design

FIGURE 1: Side view of (a) ReS₂ monolayer, (b) Janus ReSSe monolayer, (c) ReSe₂ monolayer, and (d) the hexagonal Brillouin zone of unit cell.

of new materials. The single layer crystal structure of Janus ReXY is similar to that of ReX₂ TMD, but the crystal symmetry is reduced from D_{3h} to C_{3v} [17]. In this paper, we analyzed the structure characteristics of ReS₂, Janus ReSSe, and ReSe₂, including bond lengths, and analyzed the changes under tensile and compressive strains [18]. Moreover, the three structures are direct band gap semiconductors, so their Fermi velocities are calculated, and the comparison diagram between eigenstate and strain control is drawn [19]. The phonon spectrum of the three structures has no virtual frequency, which proves that the thermodynamic stability is very good [20]. Compared with the thermodynamic stability under strain control, it is found that the thermodynamic stability under strain control is also better [21]. When it comes to band gap variation, the spin orbit coupling and energy band changes under strain are analyzed separately [22]. In other words, compressive and tensile strains are used to control the thermodynamic stability and electron behavior of such monolayer. The specific situation is analyzed in detail in Result and Discussion.

2. Method

Our calculation is based on a density functional theory [23, 24]. Generalized gradient approximation (GGA) of a function related to Perdew Burke Ernzerhof and a planar wave base group using pseudopotential [25]. Spin orbit coupling (SOC) is also applied, which affects the electron properties of a monolayer. And the electron-ion interaction is represented by the method of enhancing the wave by the projector. We calculate the band gap of the three structures. According to the Monkhorst-Pack method [26], the Brillouin region was integrated, $9 \times 9 \times 1$ K point sampling was used for self-consistent calculation, and $9 \times 9 \times 1$ is used for thermodynamic stability and electronic characteristic

calculation. A vacuum of 20 Å was provided to avoid interaction between layers.

3. Result and Discussion

3.1. Structural Properties. In the monolayers of ReS₂ and ReSe₂, the atoms are arranged symmetrically in the shape of triangular prism S-Re-S and Se-Re-Se, respectively. The symmetrical arrangement of atoms in the triangular prism shows a symmetry of D_{3h} . Moreover, ReS₂ and ReSe₂ are typical “sandwich” structures, although they are monolayers, with the same two layers of atoms holding the Re atoms sandwiched between them [27]. However, the monolayer of Janus ReSSe is formed by completely replacing S atoms with Se atoms; thus, the symmetry is reduced.

Figure 1 shows the structural side view of the monolayers of ReS₂, ReSe₂, and Janus ReSSe. For the ReS₂ monolayer, the optimized lattice parameters are $a = 6.42$ Å, $b = 6.52$ Å, and $c = 20$ Å and are consistent with the previously reported results [28, 29]. The optimized ReSe₂ lattice parameters are $a = 6.66$ Å, $b = 6.79$ Å, and $c = 20$ Å. The optimized Janus ReSSe lattice parameters are $a = 6.54$ Å, $b = 6.65$ Å, and $c = 20$ Å. The bond lengths of Re-S and Re-Se in the monolayers of ReS₂ and ReSe₂ are 2.36 Å and 2.49 Å, respectively. In the monolayer of Janus ReSSe, the bond lengths of Re-S and Re-Se are 2.36 Å and 2.49 Å, respectively. The bond angles $\angle \text{ReSRe}$ and $\angle \text{ReSeRe}$ in the ReS₂ and ReSe₂ monolayers are approximately 75.49° and 74°, respectively. These angles have changed significantly in the monolayer of Janus ReSSe; $\angle \text{ReSRe}$ is about 84.06° and is larger than the corresponding point of view in the ReS₂ monolayer, and $\angle \text{ReSeRe}$ is about 79.32° and is smaller than the corresponding point of view in the ReSe₂ monolayer. The reason for the change in bond angles is that the radius of the constituent atoms in the Janus ReSSe monolayer is different.

FIGURE 2: (a) Electronic band structure and total density of states and (b) partial density of states of ReS₂ monolayer.

FIGURE 3: (a) Electronic band structure and total density of states and (b) partial density of states of ReSeS monolayer.

3.2. Electronic Properties. The energy band structure and Fermi velocity of these monolayers were calculated. The electron band structure is plotted above. Figures 2(a), 3(a), and 4(a) show the energy band structure of the monolayers of ReS₂, Janus ReSSe, and ReSe₂, respectively, indicating that all these monolayers are direct bandgap materials. The band gap of Γ point, namely, the distance between the maximum value of valence band (VBM), and the minimum value of guide band (CBM) were observed [30]. The band gap of the

ReS₂, Janus ReSSe, and ReSe₂ monolayers calculated by GGA is 1.43 eV, 1.32 eV, and 1.25 eV, respectively.

We also calculated the partial density of the state, and the energy results of the ReS₂, Janus ReSSe, and ReSe₂ monolayers at -2 to 2 eV are summarized in Figures 2(b), 3(b), and 4(b). The ReS₂ monolayer VBM is mainly contributed by Re-d_{x²-y²} and Re-d_{x²} orbitals, while the CBM is contributed by Re-d_{x²}; however, the S atom does not contribute to the Fermi energy. Similarly, the Janus ReSSe monolayer

FIGURE 4: (a) Electronic band structure and total density of states and (b) partial density of states of ReSe₂ monolayer.

FIGURE 5: Electronic band structure of (a) ReS₂, (b) ReSSe, and (c) ReSe₂ monolayers after considering spin orbit coupling.

CBM is dominated by Re-d_{yz}, and Re-d_{x²-y²} has a partial contribution. However, the VBM state is attributed to the Re-d_{x²} orbit. A similar contribution was observed for ReSe₂, where the CBM consisted of Re-d_{yz} orbitals and the state in the VBM was dominated by the Re-d_{z²} orbit, Figure 4(b). The electron band structure with spin-orbit coupling is shown in Figure 5, which explains the strong spin-orbit splitting in the valence band. Spin orbital coupling has no effect on the bands of ReS₂ and ReSSe, while the ReSe₂ band produced a split.

3.3. Effect of Strain on Structure. Figure 6 shows the change in bond angle and bond length for ReS₂, Janus ReSSe, and ReSe₂ monolayers under compression and tensile strain [31]. Black represents the change trend of the bond length, and red represents the change trend of the bond angle.

The physical properties of these monolayers have changed under both compression and tensile strain. We calculated the bond length and bond angle changes of ReS₂, Janus ReSSe, and ReSe₂ monolayers under different Janus ReSSe, which are summarized in Figures 6(a)–6(c). For these three monolayer strains, the bond length and bond angle change properties are the same. However, the change trend of the bond length and the bond angle is opposite; the bond length decreases with the increase of the compressive strain and increases with the increase of the tensile strain. The change in the bond angle shows an opposite tendency, becomes larger with respect to an increase in compressive strain, and decreases with an increase in tensile strain.

3.4. Effect of Strain on Electronic Properties. Under the control of compressive strain and tensile strain, the electronic

FIGURE 6: The variation of bond angle and bond length under the compressive and tensile strain of (a) ReS₂, (b) Janus ReSSe, and (c) ReSe₂ monolayers.

FIGURE 7: Effect of compressive and tensile strain on band gap, D stands for direct gap and ID stands for indirect band gap.

band structures of the three monolayers have changed. Not only does the band gap change, but also the band properties shift between the direct band gap and the indirect band gap [32], as shown in Figure 7.

In order to see the electronic phase transition more accurately, we considered more points in the strain interval [33]. The ReS₂ monolayer showed a direct to indirect bandgap transition at 2% compressive strain and 6% tensile strain, as shown in Figures 7(a) and 7(b). The ReSe₂ monolayer also exhibits a direct to indirect bandgap transition at 2% compressive strain and 9% tensile strain, as seen in Figures 8(e) and 8(f). In addition, the Janus ReSSe monolayer exhibits a direct to indirect bandgap transition at 2% compressive strain and 6% tensile strain, respectively, similar to ReS₂, as shown in Figures 8(c) and 8(d). Moreover, the size of the band gap has also increased or decreased to varying degrees.

In order to visually see the change trend of the band gap under the compressive strain and tensile strain and the mutual conversion trend between the direct band and gap indirect band gap, we draw a trend chart. Purple represents the trend of ReS₂, orange represents the trend of Janus ReSSe,

FIGURE 8: Electronic band structure of (a) the ReS_2 monolayer at 2% compressive strain, (b) the ReS_2 monolayer at 6% tensile strain, (c) the Janus ReSSe monolayer at 2% compressive strain, (d) the Janus ReSSe monolayer at 9% tensile strain, (e) the ReS_2 monolayer at 2% compressive strain, and (f) ReS_2 monolayer at 6% tensile strain.

and green represents the trend of ReSe_2 . As shown in Figure 7, the band gap of ReS_2 decreases with the increase of compressive strain and decreases with the increase of tensile strain. The maximum band gap appears at 2% compressive strain. When the compressive strain is greater than 2% and the tensile strain is greater than 6%, the band gap exhibits indirect band gap, in which case the ReS_2 monolayer is a kind of indirect band gap semiconductor. And the trend of the band gap of the Janus ReSSe monolayer and the ReS_2 monolayer with strain is similar to that of the ReS_2 monolayer.

What is more, the strain phase transition point of the direct band gap and the indirect band gap of the ReS_2 monolayer is the same as that of the ReS_2 monolayer. However, the direct band gap and the indirect band gap strain phase transition point of the Janus ReSSe monolayer occur when the compressive strain is 2% and the tensile strain is 9%.

The ReS_2 single layer shows that the band gap changes are not obvious when the tensile strain and compressive strain are 0~4% and the band gap changes are not obvious when the compressive strain is greater than 4%; then the band gap changes are not obvious when the tensile strain is greater than 4%. The orange lines are shown in the figure. The band gap variation of the Janus ReSSe single layer and

ReSe_2 single layer is relatively stable, and the change of the band gap of Janus ReSSe shows a linear change, which shows a linear decrease with the increase of compressive strain and tensile strain.

4. Conclusion

The Janus ReSSe single-layer electronic band structure exhibits a direct bandgap semiconductor behavior similar to the MoSSe single layer. The band gap of the Janus ReSSe single layer is located between the band gap values of the ReS_2 and ReSe_2 monolayers. Under the influence of spin-orbit coupling, the energy band structure of ReS_2 and Janus ReSSe did not change, and the energy band structure of ReSe_2 was split. The effects of biaxial strain on the stability and electronic properties of ReS_2 , Janus ReSSe , and ReSe_2 monolayers were investigated by a density functional theory. It is found that under the influence of stress, the bond length, and bond angle of the three structures change, the bond angle decreases with the increase of tensile stress, and as the compressive stress increases, it also increases. The tensile strain increases and decreases as the compressive stress increases. Moreover, under biaxial strain, these single layers

undergo a transition between direct and indirect band gaps. These findings will provide a theoretical basis for future research and experiments.

Data Availability

Readers can find our structural parameters from the computational methods and corresponding basic data. Moreover, the corresponding basic data has been added to the new document, and readers can repeat our calculation. If you have any questions, please contact us any time.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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