Materials Research Express

PAPER

The biaxial strain induced properties of ReX₂ and ReXS (X = S, Se, Te) monolayers

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Keywords: ReX₂ monolayers, biaxial strain, electronic structure, optical properties

Abstract

In this paper, we replace the sulfur atom with other atoms based on rhenium disulfide. The monolayer is combined and adjusted on the original basis. Based on the first principle, we studied the structural, electronic and optical properties of the transition metal monolayers of ReX₂ and ReXS (X = S, Se, Te). The structure resembles a ‘sandwich’. It is worth noting that ReSeS and ReSe₂ not only retain the direct band gap properties, but also have a large band gap, when the strain changes, not only the band gap changes, but also the nature of the band gap changes with each other. So they show good optical properties, and ReSe₂ and ReSeS have stronger absorption in the ultraviolet band. The band gap opened in ReSeS can be effectively adjusted by biaxial strain, and the band gap varies between direct and indirect.

1. Introduction

Two-dimensional semiconductor materials have great application prospects in the future fields of electronics, optoelectronics and flexible electronics due to their excellent optical, electrical and mechanical properties [1]. Compared with 2H structure two-dimensional atomic crystal materials (such as MoS₂, WS₂, and MoSe₂, etc) Two-dimensional atomic crystal materials of the 1T’ structure (such as ReS₂, ReSe₂, and MoTe₂) exhibit more colorful properties due to their distinctive structural features [2, 3]. As a typical representative of the 1T’ structure two-dimensional atomic crystal material, the low symmetry lattice structure of ReS₂ gives it many excellent properties [4–6]. Such as: in-plane anisotropic optical and electrical properties, interlayer decoupling, non-layer-dependent direct band gap and other properties, these excellent properties make ReS₂ expected to be applied to the construction of new electronic devices in the future.

In recent years, researchers have done a lot of research on ReS₂. Transition metal disulfides, diselenides, transition metal oxides, and boron nitride similar to graphene are typical non-graphene two-dimensional materials, of which two-dimensional transition metal disulfides are the most attractive [7]. The research history of transition metal disulfides of bulk materials can be traced back to decades ago and is now widely used in the fields of optics, mechanics, electronics, catalysis and chemistry. However, the research on excessive metal disulfide on the two-dimensional scale is still in its infancy, and it has attracted wide attention in recent years. When the transition metal disulfide changes from a bulk material to a two-dimensional structure, the band structure of the electron changes from an indirect band gap to a direct band gap, this will greatly change the optical property and electrical properties of the transition metal disulfide [8, 9]. Not only that, but in many studies, the structure is doped with other atoms, and many good properties have been discovered, especially in terms of optoelectronic properties [10]. Associate Professor Xu Hua of Shaanxi Normal University adopted a bottom-up CVD growth method with ReO₃, S powder and Se powder as precursors, and successfully prepared a single layer of 1T’ ReSₓSe₂ (1−x) with a series of different components for the first time [11].

Inspired by the above, in this article I made some adjustments and replacements for the atoms in ReS₂. First, I constructed five structures, ReS₂, ReSe₂, ReSeS, ReTe₂, and ReTeS [12–14], and analyzed their two-dimensional structural features and electronic structures. It was found that the band gap property of the electronic structure changes between the direct band gap and the indirect band gap, and the band gap also
changes accordingly, and some structurally excellent optical properties are found. Furthermore, we add strain and electric field control on the good structure, and analysis the effect of strain electric field on the electronic structure. What’s more, also analyzed the energy band components and the atoms that contributed near the Fermi surface.

2. Method

We used the most advanced ab initio simulation based on density functional theory (DFT) [15] to study the structural and electronic properties of ReX₂ and ReXS, as implemented in VASP [16]. Generalized gradient approximations are used to exchange and correlate potentials, as proposed by hybrid functionals (HSE). The density functional method is based on the generalized gradient approximation (GGA) and local density approximation (LDA) calculation theory [17]. The cutoff energy of the plane wave is set to 300 eV, the energy accuracy is \(10^{-7} \text{ eV}\), and the maximum force allowed per atom is less than 0.01 eV Å\(^{-1}\). At the same time, we use the projector to enhance the wave method to represent the electron-ion interaction.

3. Result and discussion

3.1. The structure of ReX₂ and ReXS

DFT calculations [18, 19]. We analyzed the monolayer ReX₂ and ReXS structures, each structure contains 12 atoms, figure 1 shows, the lattice parameter of ReS₂ is \(a = 6.66 \text{ Å}, b = 6.79 \text{ Å}, c = 20 \text{ Å}\). ReSe₂ is irregular hexagon from the main view, from the side, the ReSe₂ is a ‘sandwich’ shape [20]. The top and bottom layers are Se atoms, and the middle layer is Re atoms. ReSe₂ material is not magnetic.

The lattice parameter of ReTeSe: \(a = 6.88 \text{ Å}, b = 7.02 \text{ Å}, c = 20 \text{ Å}, \) ReSeS: \(a = 6.64 \text{ Å}, b = 6.65 \text{ Å}, c = 20 \text{ Å}\), ReTeS: \(a = 6.77 \text{ Å}, b = 6.89 \text{ Å}, c = 20 \text{ Å}\) and the ReTe₂: \(a = 7.08 \text{ Å}, b = 7.22 \text{ Å}, c = 20 \text{ Å}\). We can know from the top view of figure 1, the main view and side view of the five structures are similar to ReSe₂, the yellow atom represents the sulfur element, the green atom represents the Se element, the brown atom represents the Te element, and the blue atom represents the Re element.
3.2. Electric structure of ReXS and ReX₂

Figures 2(a) and (c) are energy band structures of ReSe₂ and ReSeS respectively. As can be seen from the figure, the bandgap of the two electronic structures is a direct bandgap. ReSe₂ is a semiconductor with a bandgap of 1.25 eV, but the bandgap of ReSeS is 1.32 eV, which is larger than that of ReSe₂. And as shown as figures 2(a) and (c), we can see that the bottom of the conduction band is farther away from the Fermi surface [21].

In figures 2(b), (d) and (e), they are band structures of ReTeSe, ReTeS and ReTe₂. They are indirect bandgap semiconductor with gaps of 1.83 eV, 0.83 eV, 0.9 eV [22]. Band structures of ReSe₂ and ReSeS belong to the direct band gap, band structures of ReTeSe, ReTeS and ReTe₂ belong to indirect band gap. For optical materials, in order to make the occurrence of electronic transitions easier, generally direct bandgap semiconductors are our first choice. In contrast, carrier mobility is also much higher than indirect bandgap semiconductors [23]. Therefore, we pay attention to the various characteristics of ReSe₂ and ReSeS.

3.3. Energy component analysis of ReSe₂ and ReSeS

Relatively speaking, the direct band gap properties of ReSe₂ and ReSeS are more favorable for the study of optical properties, this band gap is more conducive to electronic transition. So we also studied the contribution of each orbital component and made a comparison. As shown below [24].

As shown in figure 3, they are the energy band component diagrams of ReSe₂ and ReSeS, in which green represents the pₓ orbital of the selenium atom, red represents the dₓᵧ orbital of the deuterium atom, blue represents the dₓz orbital of the deuterium atom, yellow represents the dₓz orbital of the deuterium atom, and purple represents the dₓz orbital of the deuterium atom. The dₓz orbital of a helium atom, dark green represents the dₓz orbital of a helium atom. It can be seen from the figures that the vicinity of the Fermi surface is mainly contributed by the dₓz orbit of the helium atom.

3.4. Effects of biaxial strain on the electric structure of ReSeS and ReSe₂

Biaxial strain were applied to ReSeS and ReSe₂ [25]. Figures 4 and 5 are part of the band diagram under biaxial strain. Figures 4(a), (b) and (d) are band diagrams under compression strain, and 4(e) are band diagrams under tensile strain. The size and property of band gap vary with strain. Figure 4(c) shows that the ReSeS is direct bandgap semiconductors. The band diagram under tensile strain shows that the position at the top of the valence band is always constant. However, under strain control, the bottom of the conduction band is getting gradually
approaches the Fermi surface. Through strain regulation, figures 4(d) and (e) indicate that the band gap transforms from direct to indirect. Figures 5(a), (b) are energy band structures of compressive strain, figures 5(d) and (e) are energy band structures of tensile strain. Figure 5(c) shows that the intrinsic ReSe₂ is a direct band-gap semiconductor, and the semiconductor properties still exist through strain regulation, but the band-gap properties change. It changes the ability of electron transition [26].

Figures 4(f) and 5(f) are bandgap trend graphs. It can be seen from the bandgap trend graph that the band gap of ReSeS changes correspondingly under strain control, the band gap becomes larger first and then decreases slowly.

Figure 3. (a) Energy bang component of ReSe₂ (b) Energy bang component of ReSeS.

Figure 4. The electric structure of ReSeS under different strain.
We add strain on the ReSeS and ReSe₂ monolayers, and have an impact on the nature of the band [27]. Figures 6(a) and (b) are energy trend diagram under the strain control. The lowest energy point is when the strain is zero.

3.5. The optical properties of ReSe₂ and ReSeS

The effect of replacing the sixth main group atom in the ReX₂ and ReXS structure was investigated to clarify its optical properties. The following is an expression of the dielectric function, where $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the real part of the dielectric function and imaginary part [28].

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

And $\varepsilon_2(\omega)$ has a concrete expression like this:

$$\varepsilon_2(\omega) = \frac{4\pi^2}{m^*\omega^2} \sum_{\nu,\nu'} \int_{\text{BZ}} d^2k \frac{2}{2\pi} |e.M(\mathbf{K})|^2 \times \delta[E_{\nu}(k) - E_{\nu'}(k) - \hbar\omega]$$

Figure 5. The electric structure of ReSe₂ under different strain.

Figure 6. (a) and (b) Energy trend diagram under the strain control of ReSeS and ReSe₂.
0 ~ 1.5 eV is the infrared range, 1.5 ~ 3.0 eV is the visible range, and more than 3.5 eV is the ultraviolet range. Figures 7(a), (c) respectively describe the imaginary part of the optical dielectric function of ReSe₂ and ReSeS. Although ReSe₂ exhibits anisotropy, we can see from the figure that along the x-axis and along the y-axis, the dielectric constants of the directions are similar, and a series of peaks are generated in the range of 1.5 to 3.0 eV. These peaks are caused by electronic transitions between Se and Re atoms, and also appear in the uv region. The maximum peak of the dielectric function appears in the high energy region, indicating that the atom is very active in this region. The z-axis peak value is around 7.0 eV, so the z-axis also contributes a lot to the optical dielectric function.

ReSe₂ and ReSeS as a sort of anisotropic material, and their band gap are directly [29, 30]. Figures 7(b), (d) is the absorption spectrum of ReSe₂ and ReSeS, the optical absorption coefficient [31]:

\[
I(\omega) = \sqrt{2} \omega [\sqrt{\varepsilon_1^2(\omega) - \varepsilon_2^2} - \varepsilon_1(\omega)]^{1/2}
\]

According to figures 7(b) and (d), the absorption coefficient of ReSe₂ and ReSeS is 1.0 eV, the absorption coefficient along the X axis is the same as the absorption coefficient along the Y axis, in other words, the absorption peak is larger and the energy range is wider, and the absorption wavelength range is correspondingly wide, and the transmission rate of the ultraviolet region is high [32]. At the same time, we found that ReSe₂ and ReSeS are very suitable for ultraviolet detectors in the range of 5.0 and 7.5 eV.

4. Conclusion

In summary, we use the FP-LAPW method to study the band structure and crystal structure of ReX₂ and ReXS (X = S, Se, Te). The band structure and optical properties of materials under strain control were studied. ReSe₂ and ReSeS are direct band gap semiconductors. In contrast, electrons are more prone to transition and have higher carrier mobility. At the same time, under the strain control, not only the band gap changes, but also the direct and indirect band gap change into each other. Optical properties of ReSe₂ and ReSeS have strong absorption in the ultraviolet band and zero absorption in the infrared band. Therefore, it would be very effective to examine its photoelectric properties in experiments for use in short-wavelength light-emitting diodes.
Acknowledgments

This work was supported by the National Natural Science Foundation of China (Grant No. 61571210, 61172028 and 11434006).

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