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COMPUTATION TO STRUCTURAL AND ELECTRONIC PROPERTIES EVOLUTION OF MONOLAYER MoS_2 INDUCED BY STRESS

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Abstract: Based on the first-principles approach of density functional theory, the evolution of the structural and electronic properties of monolayer MoS_2 due to stress is investigated by using the CASTEP module in the Material Studio software, which mainly calculates the changes of the energy band structure of monolayer MoS_2 when it is under different stresses. The calculation results show that: after applying a tensile stress of 1% lattice strain to monolayer MoS_2, the bottom point of the conduction band in its energy band remains unchanged, but the top point of its valence band will be shifted, so that its energy band structure will be transformed from a direct band gap to an indirect band gap, and with the increase of the stress up to 10%, it still maintains the indirect band gap unchanged but with the consequent decrease of the forbidden band width. On the contrary, when the single-layer MoS_2 is compressed under a compressive stress, when compressed to -10%, the single-layer MoS_2 is transformed from a semiconductor to a metal, and the absorption ability of the light in the layer will be weakened, and the corresponding reflectance will be enhanced to the point of total reflection, which is the characteristic of the metal at this time.
Keywords: MoS_2; First principles; Electronic properties; Stress

1 INTRODUCTION

In recent years, transition metal sulfides have attracted extensive interest from researchers due to their unique properties, one of which is molybdenum disulfide. One of these materials is molybdenum disulfide, which has the chemical formula MoS_2. It is a silvery-black solid that is a transition metal disulfide, and is relatively inactive compared to other transition metal disulfides because dilute acids and oxygen have essentially no effect on it. In appearance and feel, MoS_2 is graphite-like in nature and is widely used as a lubricant because of its low friction and robustness. Monolayer MoS_2 is a typical inorganic two-dimensional layered graphene-like transition metal-sulfur compounds, which has very good application prospects due to its good properties in electronics, optics, thermodynamics, chemistry, etc. It stands out from graphene led two-dimensional materials, and can even assist or replace graphene in some applications. Field effect tubes prepared using single-layer MoS_2 as the channel material have high electron mobility, large current switching ratio, and ultra-low standby power consumption. Therefore, the study of the basic structure and optical properties of monolayer MoS_2 is of great significance for the application of monolayer MoS_2 materials in optoelectronic devices [1].
Due to the difference in the electronic structure properties of monolayer MoS_2 and its body material, the MoS_2 body material is an indirect bandgap semiconductor while the monolayer material is a direct bandgap semiconductor, and the source of this difference is mainly due to the weak van der Waals force between layers in the body material. It is also therefore hypothesized that the electronic structure of monolayer MoS_2, is susceptible to change due to the interference of external factors[2]. For this reason, in this paper, we apply the first principle method to realize the regulation of the electronic structure by applying the stress (changing the lattice constant) within the layers, and analyze and study the electronic properties of monolayer MoS_2 by comparing with the energy band diagrams.

2 MODELING AND CALCULATION METHODS

2.1 Model

MoS_2 is a typical lamellar material with hexagonal honeycomb structure, each MoS_2 monolayer is stacked by Mo atoms in the center layer and S atoms in the upper and lower layers, presenting an S-Mo-S-like sandwich structure that is very stable, and the Mo atoms in the middle layer and the six S atoms are combined to form a two-dimensional atomic crystal by covalent bonding between them, which makes the monolayered MoS_2 nanomaterials have a very stable structure[3]. Since the layers of molybdenum disulfide are bonded to each other by a weak van der Waals force, the coupling is very weak, and thus it is extremely easy to be separated into independent monolayers[4], as shown in Figure 1. In this paper, we study a single layer of MoS_2,the specific structure is shown in Figure 2.

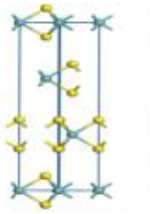


Figure 1 Structure of MoS_2 Body Material

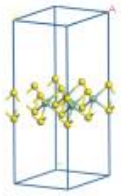


Figure 2 Structure of Single Layer MoS_2

2.2 Calculation Methods

In this study, the CASTEP module in the first principles business software Materials Studio, which is based on density functional theory, is used for the calculation about the energy band structure[5]. In the process of calculating the energy band structure, the MoS_2 model is firstly established in Materials Studio, and the monolayer is intercepted on the bulk structure, and then the total energy of the monolayer MoS_2 is calculated, and the structure of the monolayer MoS_2 is optimized, which is made to reach the optimal energy band structure and the most stable state by varying the lattice constants of the monolayer MoS_2 and the thickness of the monolayer, and then by varying the molybdenum disulphide layer The magnitude of the internal stress, which is achieved by changing the lattice constant, is observed for the energy band structure and its properties are analyzed.

3 CALCULATION RESULTS AND DISCUSSION

3.1 Structural Optimization

After intercepting the monolayer of molybdenum disulfide, it is firstly necessary to optimize its structure, and the optimization mainly includes two aspects, which are the optimization of lattice constants and the optimization of monolayer thickness. And on this basis, the electronic structure calculation is carried out, so as to obtain the energy band diagram of the monolayer MoS_2 crystals, and then through the observation of the energy band diagram, the forbidden band widths when applying different degrees of stress within the monolayer of molybdenum disulfide layer are analyzed and the structure type is derived.
The relational equations for their lattice constants and energies are given below:

$$E = 7.3111a^2 - 46.61a - 2421 \tag{1}$$

Increasing or decreasing the thickness of the monolayer is carried out with the optimal lattice constant so that the force equilibrium can be maintained even in the numbered straight plane. As shown in Figure 3-4, it can be seen that the correlation coefficient = 0.9826 i.e. very close to 1, indicating that the fit is good and the monolayer thickness-energy relationship has:

$$E = 5.1266d^2 - 30.356d - 2448.6 \tag{2}$$

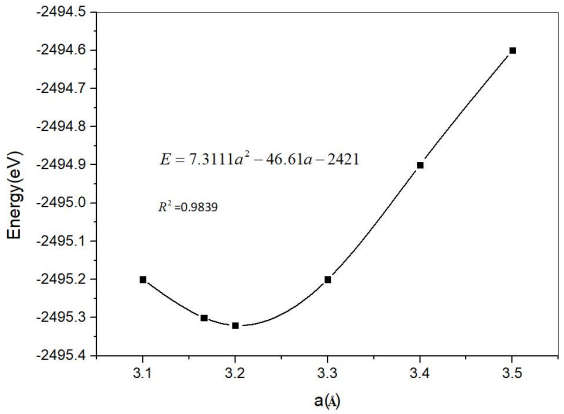


Figure 3 Trend of Lattice Constant a for MoS_2 Lattice Structure

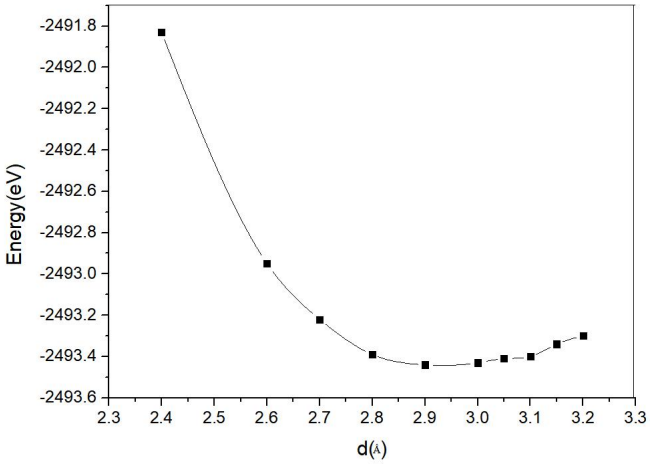
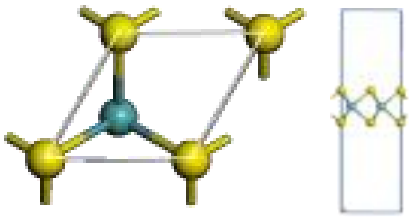


Figure 4 Trend of MoS_2 Lattice Structure Monolayer Thickness *d*

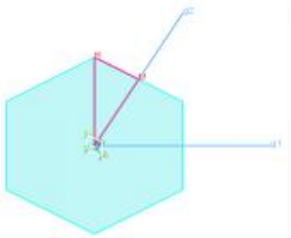
3.2 Regulation of Electronic Structure

According to the energy band diagram, we can determine whether the MoS_2 structure belongs to a conductor, semiconductor or insulator, in which the semiconductor type we can analyze whether it is a direct bandgap semiconductor or indirect bandgap semiconductor according to the energy band structure, which we can know by reading the value of the bandgap in the energy band diagram as well as the movement of each bandgap[6].

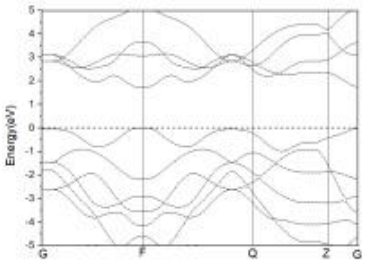
For example, Figure 5(a) shows the monolayer MoS_2 structure, at this time, the energy of the monolayer MoS_2 structure is the lowest, and the forces between the atoms are also balanced, which is the most stable state. The coordinate position of the high symmetry point in the Brillouin zone in Figure 5(b) has been constant, and the coordinates are G(0,0,0), F(0,0,0.5), Q(-0.333,0.667,0.500), Z(-0.333,0.667,0), and G(0,0,0) in that order, and it can be seen that the Fermi energy levels do not intersect with the conduction bands, so it is the semiconductor state. Figure 5(c) shows the energy band diagram of the complete structure of monolayer MoS_2, in which the Fermi energy levels are between the valence band and the conduction band, which do not intersect but are on the same wavevector, so it can be known that the monolayer MoS_2 is a direct bandgap semiconductor.



(a) Structure of monolayer MoS_2



(b) High symmetry points and path diagrams in the Brillouin zone



(c) Energy band diagrams

Figure 5 Structures of MoS_2

4 VARIATION OF ENERGY BANDS WITH STRESS

3.1 Tensile Stresses on Monolayer MoS_2

Figure 6 shows the top view of the monolayer MoS_2 crystal structure without applied strain. After we optimized the

monolayer structure, we applied strain in the a_1, a_2 direction, respectively, resulting in a lattice strain (ε) defined as the ratio of the change in the lattice constant, Δa , to the lattice constant, ($\varepsilon = \Delta a / a$)[7], a process that is achieved by directly altering its lattice constant.

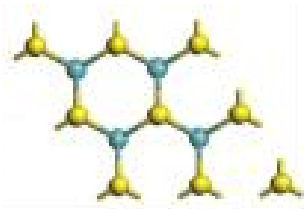
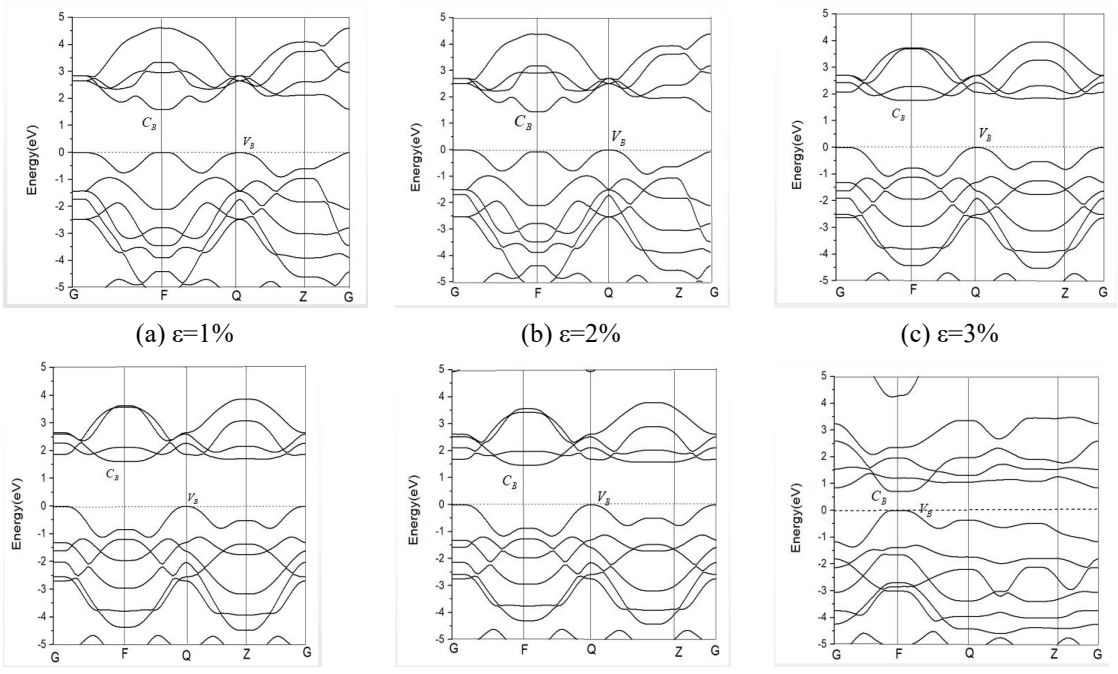


Figure 6 Top View of Single Layer MoS_2 Crystal Structure

From the energy band structure of monolayer molybdenum disulfide, it can be seen that when no strain is applied, the monolayer MoS_2 is a direct bandgap, the lowest point of the conduction band and the highest point of the valence band are at the point F, and the value of the bandgap is 1.612 eV, and the width of the forbidden band is 1.654 eV. When the stress is applied to the monolayer MoS_2, the highest point of the valence band is shifted but the lowest point of the conduction band is still at the point F. Therefore, we keep changing the value of ε with 1%, 2%, 3%, 4%, 5%, 10%, -1%, -2%, -3%, -4%, -5%, -10%, to observe the changes in the energy band structure and to summarize the conclusions.
When a 1% strain is applied to the MoS_2 monolayer, the band gap value becomes 1.598 eV, and the valence band position is at -0.001, at which time the molybdenum disulfide is transformed from a direct band gap semiconductor to an indirect band gap semiconductor; when a 2% strain is applied to the layer, the band gap value becomes 1.443 eV, and the valence band position is at -0.006, which is still the type of an indirect band gap semiconductor. When 3% strain is applied to the layer, the band gap value becomes 1.142eV, with the valence band at -0.0089; when 4% strain is applied to the layer, the band gap value becomes 1.011eV, with the valence band at -0.007; when 5% strain is applied to the single layer of molybdenum disulphide, the band gap value becomes 0.887eV, with the valence band at 0.013eV, and the positions of the bottom of the conduction band and the top of the valence band remain deviated. The bottom of the conduction band and the top of the valence band are still deviated; when 10% strain is applied, the bandgap value becomes 0.707eV, and the valence band is at -0.001eV, keeping the indirect bandgap semiconductor characteristics unchanged. The corresponding energy band diagrams for the stress change process from 1% to 10% are shown in Figure 7 (a)-(f) below.



(a) ε=1% (b) ε=2% (c) ε=3%

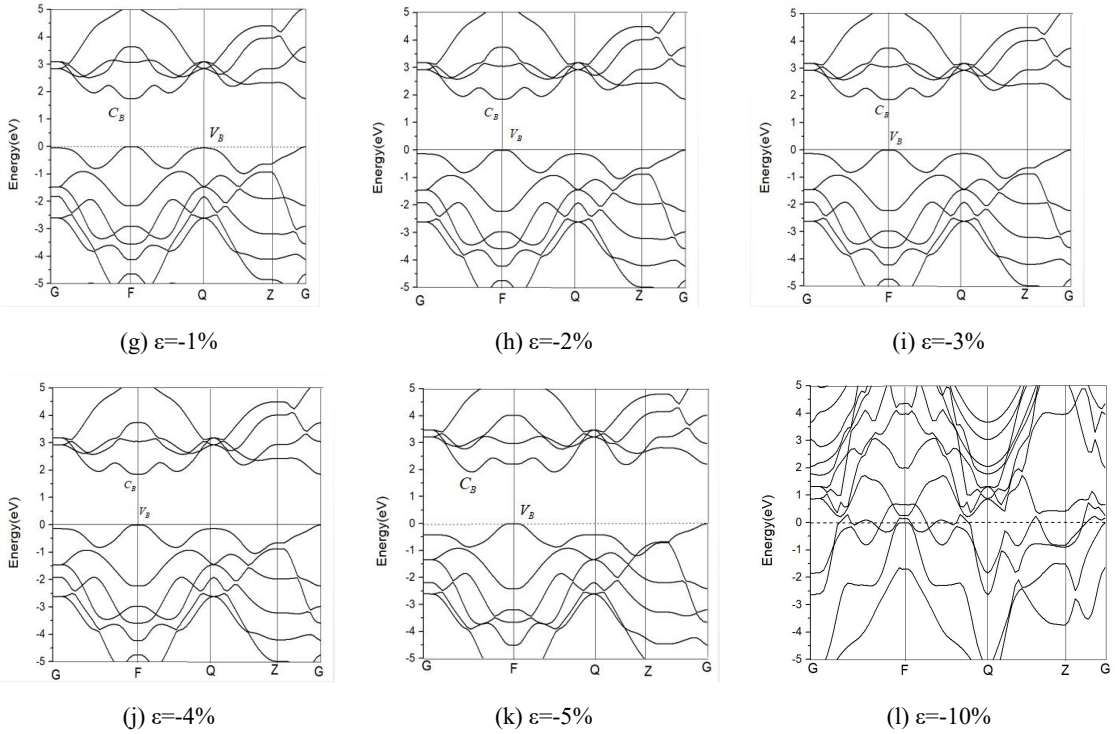
(d) ε=4% (e) ε=5% (f) ε=10%

Figure 7 Lattice Strain of 1% to 10%

3.2 Compressive stressing of monolayer MoS_2

When a strain of ε-1% is applied to the MoS_2 layer, the bandgap value becomes 1.748eV, and the direct bandgap semiconductor type of molybdenum disulfide remains unchanged; when a strain of -2% is applied to the molybdenum disulfide monolayer, the bandgap value becomes 1.852eV; when a strain of -3% is applied, the bandgap value becomes

1.942eV, and when a strain of -4% is applied to the layer, the bandgap value becomes 1.930eV. When -3% strain is applied, the band gap value becomes 1.942eV, and when -4% strain is applied to the layer, the band gap value becomes 1.930eV, and the two energy band diagrams still keep the direct band gap semiconductor type; when -5% strain is applied, the band gap value becomes 1.914eV, and the position of the valence band is shifted, and the molybdenum disulfide changes into an indirect band gap semiconductor; when -10% strain is applied, the overlapping of conduction and valence bands occurs between the conduction and the valence bands of the energy band structure of the single-layer MoS_2, and the forbidden band disappears. overlap, the forbidden band disappears, and electrons can reach the conduction band without obstacles, at which time molybdenum disulfide is transformed from a semiconductor to a metal[8]. The results show that the different sensitivities of the intrinsic energies of the F-points in the Brillouin zone to the pressure are the root cause of the transformation of the energy band structure of monolayer molybdenum disulfide. The corresponding energy band diagrams for the change of stress from -1% to -10% in the layer are shown below in Figure 8 from (g) to (l).



(g) ε=-1% (h) ε=-2% (i) ε=-3%

(j) ε=-4% (k) ε=-5% (l) ε=-10%

Figure 8 Lattice Strain of -1% to -10%

Therefore, through the calculation in the Materials studio, it can be verified that the bandgap value will indeed decrease with the increase of the stress in the layer, so its forbidden bandwidth will gradually decrease, at this time, the single layer of molybdenum disulfide will be transformed from a direct bandgap semiconductor to an indirect bandgap semiconductor, because there is a semiconductor type of transformation, so the difference in the bandgap value will also be different, and therefore it is not a linear The difference in band gap value decreases differently because of the semiconductor type transition, so it is not a linear increase or decrease graph. Instead when a decreasing stress is applied to the monolayer molybdenum disulfide, the band gap value first increases and then decreases and finally decreases to 0. The monolayer molybdenum disulfide undergoes a change from a semiconductor to a metal[9].

5 CONCLUSION

In this paper, based on the calculation of the first principle of density functionality, it is concluded that the monolayer MoS_2 is a direct bandgap semiconductor with a forbidden bandwidth of 1.654 eV by applying the CASTEP module in the Materials studio software.The effect of tensile strain or compressive strain on the energy band structure of the monolayer MoS_2 is investigated, and when an increase of 1% is applied to the monolayer MoS_2, the monolayer MoS_2 will be transformed from a direct bandgap semiconductor to an indirect bandgap semiconductor. At this point, molybdenum disulfide transforms from a direct band gap to an indirect band gap, and subsequently, during the continuous stressing of the monolayer MoS_2, the monolayer MoS_2 has remained an indirect band gap semiconductor unchanged, and the forbidden bandwidth is decreasing with the increase of the stress. The reason for such a transition is due to the shift in the valence band position and the energy change at the F-point is not as sensitive to the stress[10]. On the contrary, when the monolayer MoS_2 is subjected to a reduced stress of 1%, the molybdenum disulfide is still a direct bandgap semiconductor, and when the reduced stress is -4%, the monolayer MoS_2 will be converted from a direct bandgap to an indirect bandgap, and when the reduced stress reaches -10%, a semiconductor-to-metal transition will take place, corresponding to the enhancement of reflectivity, reaching the point of total reflection, which then exhibits

the characteristics of a metal.

COMPETING INTERESTS

The authors have no relevant financial or non-financial interests to disclose.

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