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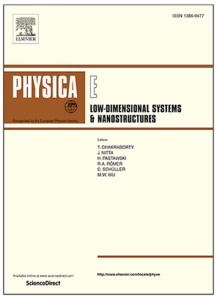

Strain effects on the electronic and optical properties of Van der Waals heterostructure MoS_2/WS_2: A first-principles study

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Strain effects on the electronic and optical properties of Van der Waals heterostructure MoS_2/WS_2: A first-principles study

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Abstract

In the present work, the effect of biaxial and uniaxial strains on the electronic and optical properties of heterostructure MoS_2/WS_2 has been studied by density functional theory. Our numerical calculations demonstrate that the heterostructure MoS_2/WS_2 is an indirect semiconductor with a type-II band alignment and its energy gap is 1.45 eV. Besides, the semiconductor-metal transition can be found at large biaxial strain of 14% in the van der Waals heterostructure MoS_2/WS_2. Influence of the strain engineering on the optical spectra of the heterostructure MoS_2/WS_2 are also considered in this work. Our calculations indicate that, while the effect of uniaxial strain on the optical properties is quite weak, the optical parameters of the heterostructure MoS_2/WS_2 depend strongly on the biaxial strain. Our predicted results may be a reference for future experimental and theoretical studies of the heterostructures.

Key words: Van der Waals heterostructure, strain engineering, electronic and optical properties, DFT calculations

1 Introduction

Since graphene was discovered in 2004 [1], a new era for two-dimensional (2D) materials has been opened. Due to its outstanding and exotic properties, graphene has attracted many theoretical and experimental researchers. However, the biggest drawback of graphene is that it has zero energy gap, which makes graphene very difficult to apply in electronic devices and competitive with existing silicon devices. In parallel with overcoming the limitations of graphene, scientists have also searched for alternative materials and the transition metal dichalcogenides (TMDs)

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are one of the 2D materials families believed to have superior properties expected to have many applications in nanotechnology [2–7].

Contrary to graphene, a semiconductor with zero bandgap, monolayer TMDs are semiconductors with natural bandgap [8]. Also, in the bulk structure, the layers of TMDs are kept together by weak van der Waals forces [9]. Therefore one can be easily separated them into single layers by conventional methods [10]. In parallel with the study of the properties of monolayers TMDs materials, the successful isolation of diverse 2D layered materials recently [11, 12] raised the possibility of creation of new van der Waals heterostructures which offer many possibilities by stacking 2D materials [13–16]. The previous study indicated that heterostructure based on the transition metal dichalcogenides MX_2, such as MX_2/graphene which is synthesized by chemical vapor deposition (CVD) [17], is suitable for applications in photovoltaic devices. Kis and co-workers have also demonstrated that the MoS_2/graphene heterostructure can be used to build memory cells [18] or $WS_2/MoSe_2$ heterostructure is predicted to be very useful for applications in solar cell [19] and photodetectors [20]. Recently, MX_2/MX_2 heterostructures such as $WSe_2/MoSe_2$ or WS_2/MoS_2 heterostructures have been synthesized and investigated by both Raman spectroscopy and photoluminescence [6, 19]. In fact, it is experimentally unknown in this new type of van der Waals heterostructures whether the optical transitions will be indirect or direct and the stacking of these 2D materials allows considering an unlimited number of architecture creating new devices to imitate the properties of standard materials. Previous computational works have demonstrated that we can tune and control the electronic and optical properties of 2D materials by strain engineering or eternal electric field [21–24]. Recently, heterostructures based on TMD monolayer have also been considered by density functional theory (DFT) [25–27].

The physical properties, especially optical and electronic properties, of the het-

erostructures can be drastically altered by strain engineering. In the present work, we investigate the electronic properties of MoS_2/WS_2 hetero-bilayers and the influence of biaxial ε_{bia} and uniaxial strain along with the armchair/zigzag direction $\varepsilon_{arm/zig}$ on the electronic properties and optical characteristics of the vertical MoS_2/WS_2 heterostructure using DFT calculations. We focus on the effect of strain engineering on the band gap and the basic optical characteristics of the vertical MoS_2/WS_2 heterostructure.

2 Model and methods

The electronic and optical properties of MoS_2/WS_2 in this work have been investigated using the full-potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2K simulation package [28]. In the present work, we used the generalized gradient approximation (GGA) based on the Perdew-Burke-Ernzerhof (PBE) parameterization. Muffin-tin radii R_{MT} were chosen to avoid the overlap between atomic spheres. After the convergence test, we choose the $R_{MT} * K_{max} = 7.5$, where K_{max} is the maximum modulus for the reciprocal lattice vectors. In our calculations, we used the $G_{max} = 12$ and 500 k-points in the first Brillouin zone (BZ) for both optical and electronic properties. The total energy at the equilibrium state of the MoS_2/WS_2 hłtrostructure is -43625.3954 eV. The c/a ratio and volume were optimized using the 2D optimize package suggested by Reshak and Morteza [29]. We know that the van der Waals (vdW) interactions in layered 2D vdW heterostructures cannot be accurately described by traditional DFT methods. Therefore, in order to solve this problem, in this work, the long-range weak vdW interaction in the MoS_2/WS_2 heterostructure have been calculated through the DFT-D2 method proposed by Grimme [30]. Also, to avoid the interaction between two adjacent periodic slabs, a large vacuum space of 20 Å in

the direction perpendicular to the 2D surface of the heterostructure is applied.

In this study, we investigate the optical properties of the heterostructure MoS_2/WS_2, focusing on the basic optical characteristics only. The dielectric function can be expressed as $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, where $\varepsilon_1(\omega)$ is the real part of the dielectric function which can be gained via the Kramers-Kronig transformation from the imaginary part $\varepsilon_2(\omega)$. The imaginary part $\varepsilon_2(\omega)$ is given by [31]

$$\varepsilon_2^{ij}(\omega) = \frac{4\pi^2 e^2}{Vm^2\omega^2} \sum_{knn'\sigma} \langle kn\sigma|p_i|kn'\sigma\rangle\langle kn'\sigma|p_j|kn\sigma\rangle \times f_{kn}(1-f_{kn'})\delta(E_{kn'}-E_{kn}-\hbar\omega), \tag{1}$$

where V is the volume of the unit cell, ω is the angular frequency of the incident photon, e and m are respectively the charge and mass of the electron, p is the momentum operator, $|kn\sigma\rangle$ is the wave function with the eigenvalue E_{kn}, and f_{kn} is the Fermi distribution function.

The absorption coefficient $\alpha(\omega)$ and the electron energy loss spectrum $L(\omega)$ can be also expressed via the parts of $\varepsilon(\omega)$ as [32]

$$\alpha(\omega) = \frac{\sqrt{2}\omega}{c}\left[\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right]^{1/2}, \tag{2}$$

$$L(\omega) = -Im(\varepsilon^{-1}) = \frac{\varepsilon_2(\omega)}{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)}. \tag{3}$$

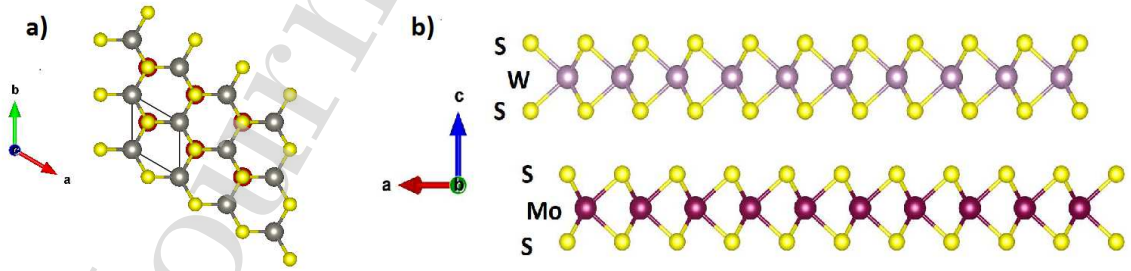

Fig. 1. (a) Top view of atomic structure of MoS_2/WS_2 heterostructure, (b) vertical stacking of MoS_2 and WS_2 monolayers.

3 Results and discussion

3.1 Electronic properties

Before investigating the electronic properties of considered here heterostructures, we first performed several tests on the convergence of the total energy of each monolayer as a function of *k*-point mesh, cut-off energy and lattice parameters for different *k*-point meshes and cut-off energies. From these tests, we can obtain the accuracy of the lattice parameter of MoS_2 and WS_2 monolayers, respectively, are $a_0(MoS_2) = 3.19 \pm 0.04$ and $a_0(WS_2) = 3.18 \pm 0.05$. We find that these values are in good agreement with the previous theoretical reports [33–35] and experimental measurements [36, 37]. Analyzing the aforementioned data, we believe that our choice of the PBE exchange-correlation functional for current systems is appropriate, and a general idea of the trends can anticipated from our results. The MoS_2 and WS_2 monolayers can form several different stacking conformations. The most stable heterojunction structure is C7 stacking which is the stacking of bulk MoS_2 and WS_2 [38]. Such an affirmation is confirmed by many theoretical reports [38–42]. In the present study, we focus on the C7 stacking as shown in Fig. 1. From the atomic structure of the MoS_2/WS_2 heterostructure as shown in Fig. 1, we can see that each bilayer of MoS_2/WS_2 is composed of a plane of molybdenum atoms or tungsten sandwiched between two planes of sulfur atoms as shown in Fig. 1(b). The MoS_2 and WS_2 monolayers in heterostructure are held together by weak van der Waals forces. At equilibrium, the lattice constant MoS_2/WS_2 heterostructure is $a = 3.197$ Å.

The total energy, as illustrated in Fig.2 demonstrates that the MoS_2/WS_2 heterostructure is stable at the equilibrium state. Effect of strain engineering on the total energy of the heterostructure is shown in Fig. 2. Figure. 2 indicates that the

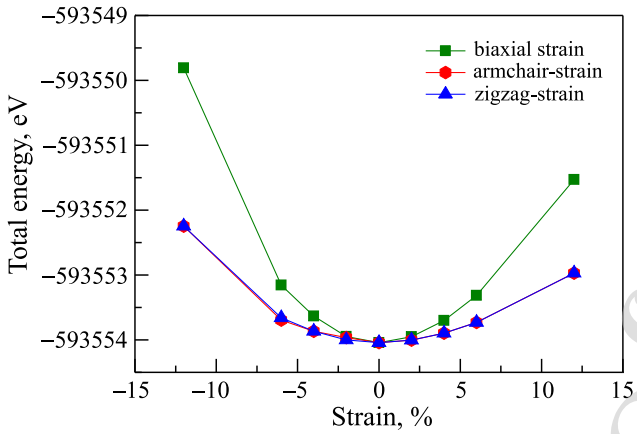

Fig. 2. Dependence of total energy of MoS_2/WS_2 heterostructure on strain engineering.

effects of the uniaxial strains along the zigzag ε_{zig} and armchair ε_{arm} directions on the total energy of the system is quite small. The change in total energy under different uniaxial strains is small of about 0.027 eV at the compression of 4%. This result is in agreement with previous works on other compounds [43, 44], which is about 4.4 times smaller than the difference caused by uniaxial and biaxial strains (about 0.117 eV). The biaxial strain affecting the total energy is larger than the case of the uniaxial strain. However, the effect of strain on the total energy is generally quite small, especially in small strain limits. Our calculations show that the band structure of MoS_2/WS_2 heterostructure at equilibrium shows an indirect band gap of 1.45 eV [Fig. 3(a)]. Our calculated results also demonstrated that the band gaps monolayers MoS_2 and WS_2 are respectively 1.72 eV and 1.85 eV. In addition, both the valence band maximum (VBM) and the conduction band minimum (CBM) of the monolayer MoS_2 are lower than that of the monolayer WS_2, therefore MoS_2/WS_2 heterostructure is a semiconductor with type-II band alignment with the VBM and CBM locating in two separate monolayers. This estimation is in agreement with previous experimental [6] and theoretical reports [39, 45]. Although the MoS_2/WS_2 heterostructure is an indirect semiconductor, we find that, as shown in Fig. 3(a), the energy difference between the VBM at the Γ-point and the energy of

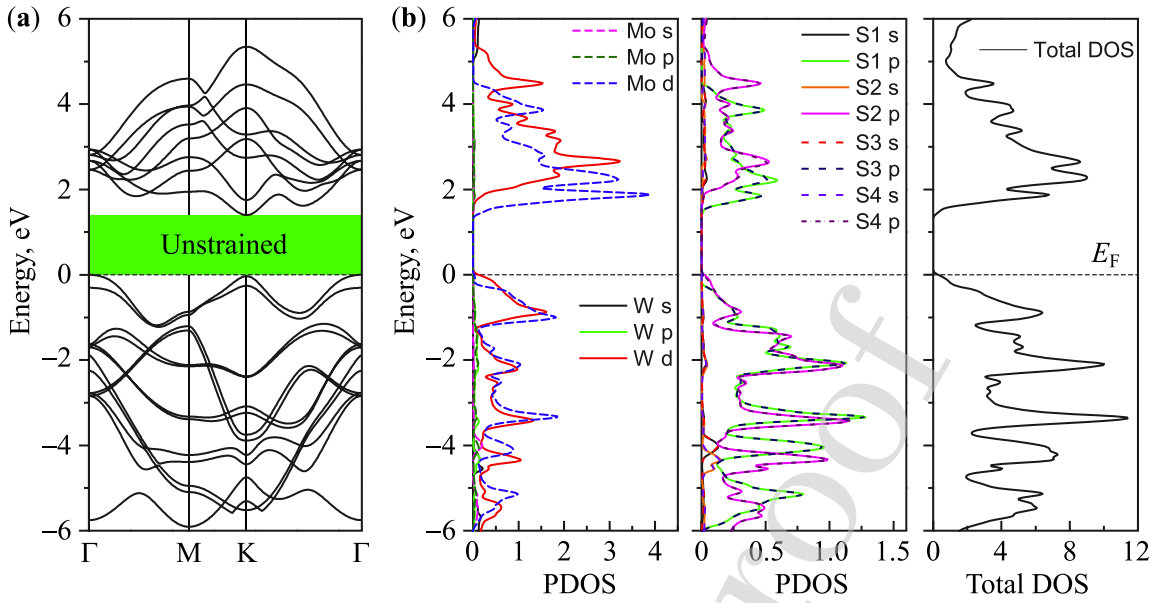

Fig. 3. Band structure (a) and density of states (b) of MoS_2/WS_2 heterostructure at equilibrium.

the highest subband of the valence band is very tiny at the K-point. Therefore, we believe that external impacts, such as strain, can alter the VBM position leading to indirect–direct band gap transition. Figure 3(b) illustrated the partial density of states (PDOS) of the heterostructure at the equilibrium state. We can see that the Mo-d and W-d contribute significantly to the valence and conduction bands of the MoS_2/WS_2 heterostructure.

Note that a vertical stacking of MoS_2 and WS_2 monolayers, without depletion region, leads to a rapid interlayer charge transfer [46, 47]. In addition, charge carriers are localized largely in separate layers and manifests a vertical p–n junction out-of-plane [48, 49]. In MoS_2/WS_2 hetero-bilayers, electrons (holes) are confined to the MoS_2 (WS_2) monolayer. One showed that the charge-transfer time in MoS_2/WS_2 heterojunction is in femtosecond scale. It is extremely smaller than that in MoS_2 and WS_2 monolayers [47]. The investigated MoS_2/WS_2 heterojunction shows a lower band gap than the bands of monolayers. This electron–hole vertical separation will eliminate the electron–hole pairs recombination and prolong the

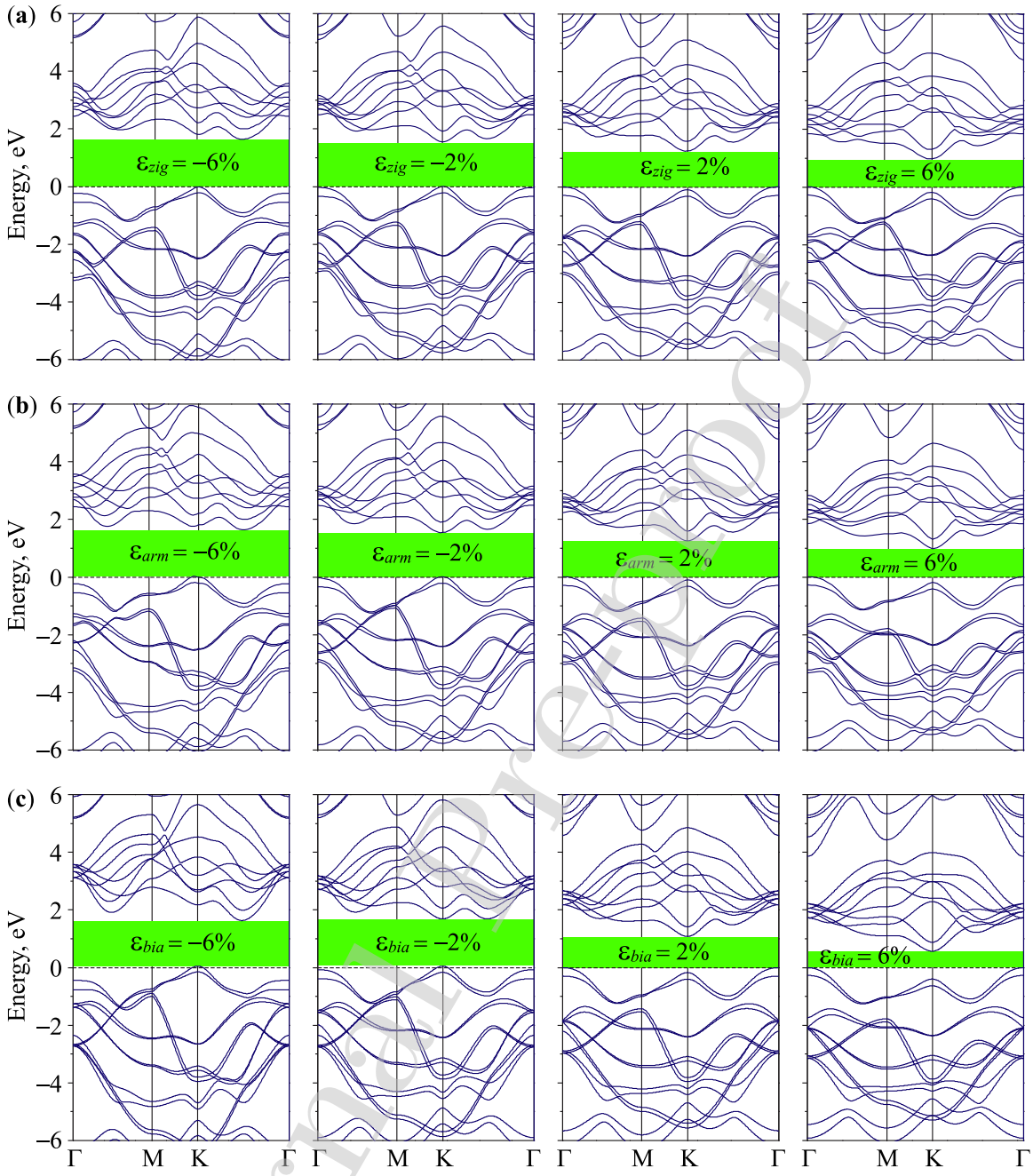

Fig. 4. Band structure of MoS_2/WS_2 heterojunction under different levels of uniaxial strain along zigzag direction ε_{zig} (a) and armchair direction ε_{arm} (b) and biaxial strain ε_{bia} (c).

lifetimes of inter-layer excitons compared to individual monolayers. Figure 3(b) shows the partial density of states (PDOS) of the MoS_2/WS_2 heterobilayer at the equilibrium state. We can see that the VBM is greatly donated from the W-d orbital in the WS_2, while the CBM is highly donated from the Mo-d orbital in the MoS_2

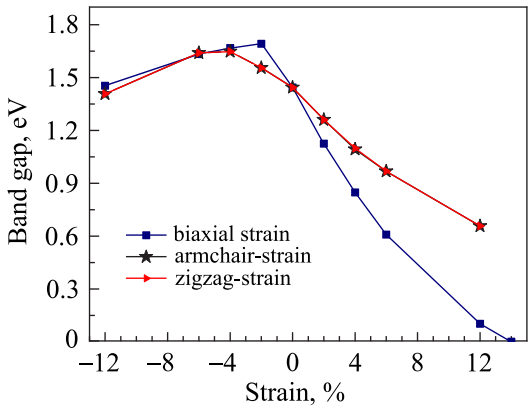

Fig. 5. Dependence of energy gap of the MoS_2/WS_2 heterostructure on the strain engineering.

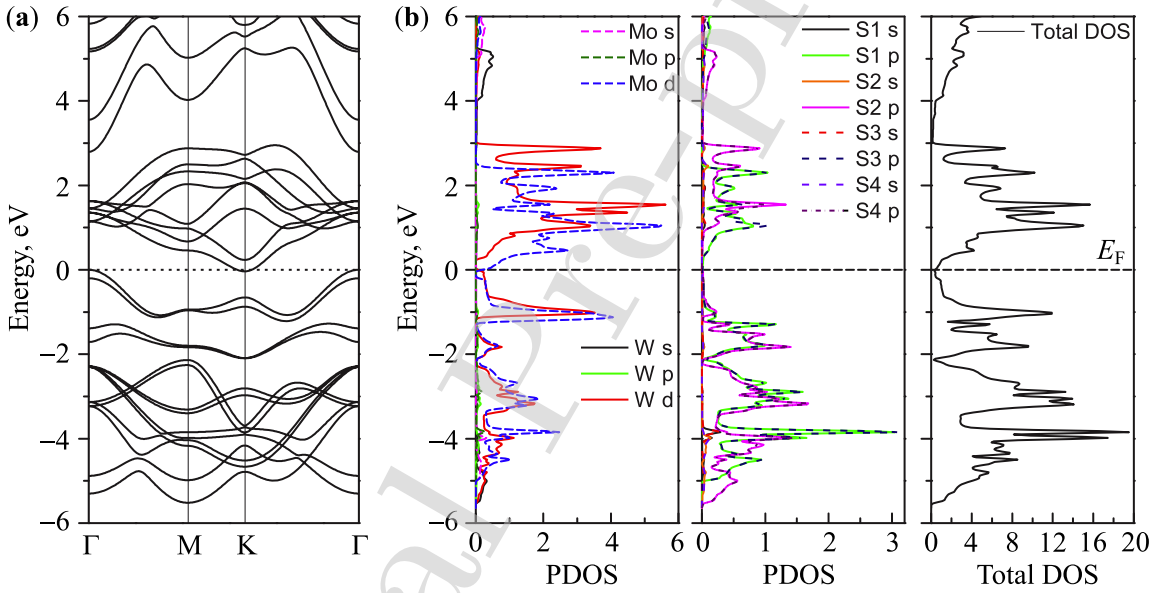

Fig. 6. Band structure (a) and density of states (b) of the MoS_2/WS_2 heterostructure at $\varepsilon_{bia} = 14\%$.

layer. In the presence of strain, the CBM can be shifted toward the Fermi level due to the applied strain. This shifting of the CBM leads to a reduction in the energy gap of the MoS_2/WS_2 heterostructure as shown in Fig.4. Also, from Fig. 4 we can see clearly that the uniaxial strain has not only changed the energy but also changed the basic properties of the material, namely the MoS_2/WS_2 heterostructure becomes a direct semiconductor at $\varepsilon_{arm/zig} = \pm 2\%$. However, in larger uniaxial strains, the

shifting of the CBM and VBM causes the MoS_2/WS_2 heterostructure to return to the indirect semiconductor. The biaxial strain did not result in the indirect–direct bandgap transition as in the case of uniaxial strain. Influence of the strain engineering on the band gap of the MoS_2/WS_2 heterostructure is shown in Fig. 5. There is no difference clearly in energy gap in two cases of uniaxial strains. Compared to uniaxial strain, the energy gap of the MoS_2/WS_2 heterostructure depends greatly on biaxial strain ε_{bia}, particularly in the tensile ε_{bia} case. Interestingly, the energy gap of the MoS_2/WS_2 heterostructure drops to zero when the biaxial strain $\varepsilon_{bia} = 14\%$ is applied. It means that the semiconductor–metal phase transition was observed in the MoS_2/WS_2 heterostructure at large tensile biaxial strain. Band structure and PDOS of the MoS_2/WS_2 heterostructure at transition point of $\varepsilon_{bia} = 14\%$ is shown in Fig. 6. As shown in Fig. 6, the CBM and VBM are in the Fermi level $E = 0$ at the K- and Γ-point, respectively. The semiconductor-metal phase transition in MoS_2/WS_2 heterostructure is considered as one of the key factors for large application mainly in electro-mechanical actuators and sensors.

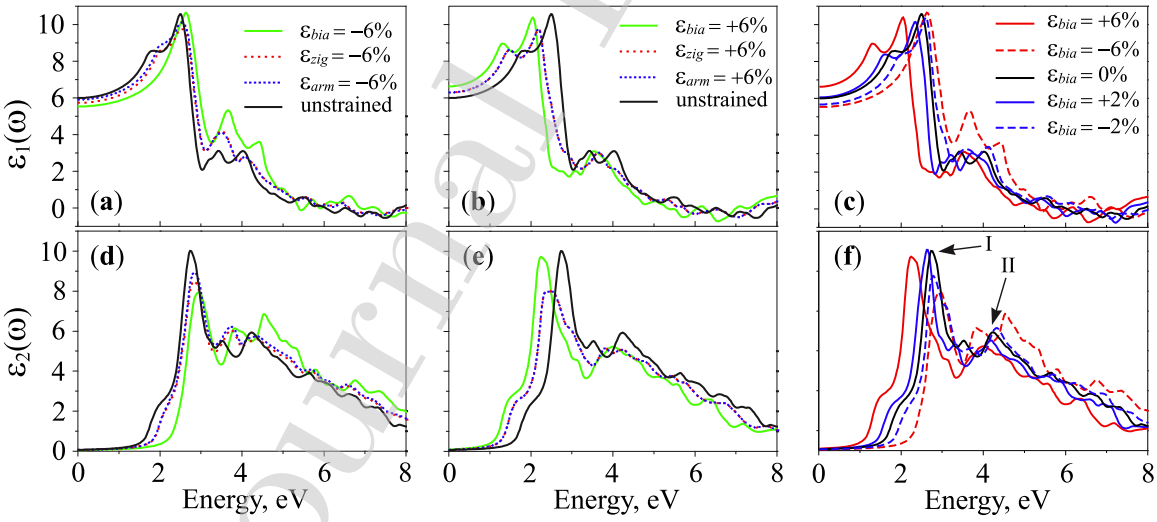

Fig. 7. Real $\varepsilon_1(\omega)$ and imaginary $\varepsilon_2(\omega)$ parts of $\varepsilon(\omega)$ in the xy-plane of MoS_2/WS_2 under uniaxial and biaxial strains of -6% (a) and $+6\%$ (b) and under different levels of biaxial strain (c).

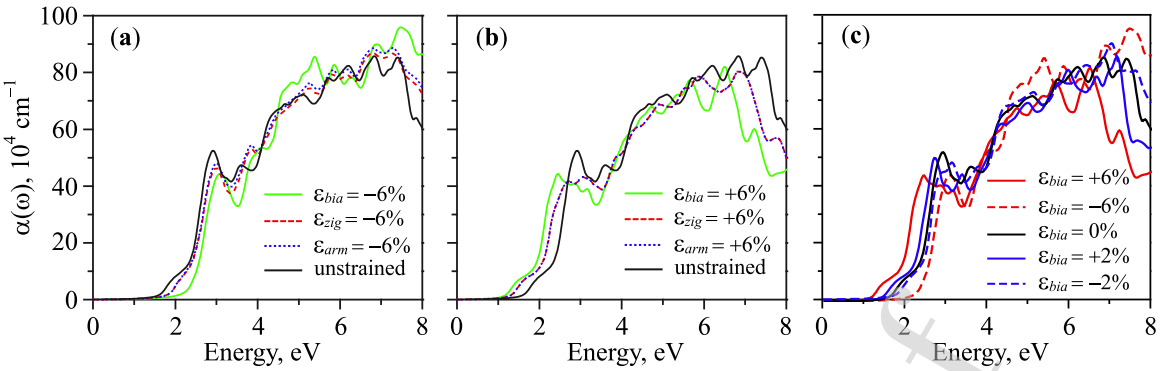

Fig. 8. Absorption coefficient $\alpha(\omega)$ of MoS_2/WS_2 heterostructure under strains of -6% (a) and $+6\%$ (b) and under different levels of biaxial strain (c).

3.2 Optical properties

In this part, we will briefly study the influence of the uniaxial and biaxial strains on the optical property of vertical heterojunction MoS_2/WS_2. We first calculate the parts of the $\varepsilon(\omega)$ of vertical heterojunction MoS_2/WS_2 using Eq. (1). The parts of the $\varepsilon(\omega)$ of the MoS_2/WS_2 without and with strain engineering is shown in Fig. 7. Computational results demonstrate that both $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ parts of the $\varepsilon(\omega)$ depend quite strong on the strain engineering, especially biaxial strain ε_b. Focusing on the biaxial strain case, in Figs. 7(c) and 7(f) we show respectively the $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ parts under different levels of the ε_{bia}. It can be seen that in Fig. 7(f), the position of the peaks I and II is redshifted. Also, we can see that the peak I intensity in the case of tensile strain is greater than that of the compressive strain, and vice versa, the peak II intensity is increased by compressive biaxial strain.

The calculated strain-dependent optical absorption $\alpha(\omega)$ spectra are presented in Fig. 8. It shows that the strain considerably affects the optical absorption of vertical heterojunction MoS_2/WS_2. In the considered range of energy from 0 to 8 eV, the maximum of $\alpha(\omega)$ of the MoS_2/WS_2 heterostructure is about 7.5 eV. As shown in Fig. 8(c), the effect of strains, especially biaxial strain, on the absorption coef-

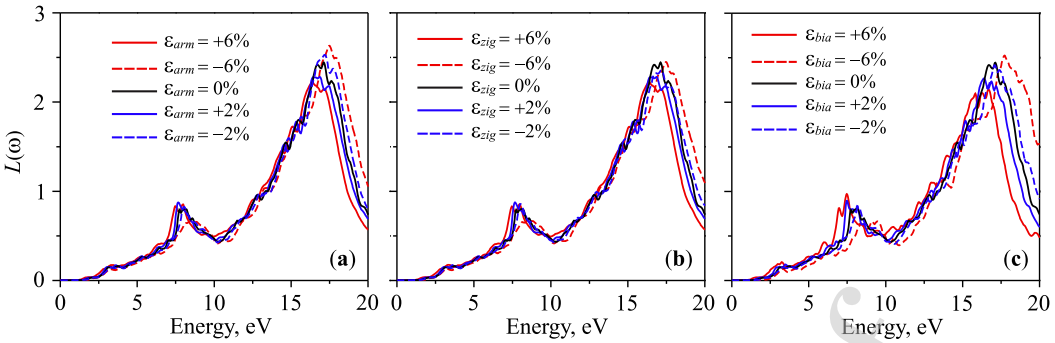

Fig. 9. Electron energy loss spectrum $L(\omega)$ of MoS_2/WS_2 under different levels of ε_{amr} (a), ε_{zig} (b), and ε_{bia} (c).

ficient is outstanding in the high energy region, higher than 6 eV. The influence of the strains on the energy loss spectra of electrons $L(\omega)$ is shown in Fig. 9. We can see that the $L(\omega)$ depends slightly on the uniaxial strain but it is greatly affected by the ε_{bia} as shown in Fig. 9(c). It is clear that the influence of the biaxial strain on the optical spectra of the vertical heterojunction MoS_2/WS_2 becomes more pronounced compared to the uniaxial strains. We believe that the optical spectra, as well as electronic properties of vertical heterojunction MoS_2/WS_2, are quite sensitive to biaxial strain which is an important characteristic for its applications in the optoelectronic and electro-mechanical devices.

4 Conclusion

In summary, we examined the influence of strains on optoelectronic properties of vertical heterojunction MoS_2/WS_2. Our calculations show that while MoS_2 and WS_2 monolayers are direct semiconductors, the vertical stacking MoS_2/WS_2 heterostructure is an indirect semiconductor and the charge carriers in this heterostructure are widely localized on different layers. At equilibrium, the MoS_2/WS_2 heterostructure is an indirect semiconductor with type II band alignment and its band gap can be tuned and controlled by a uniaxial and biaxial strain. The optical spectra

of the MoS_2/WS_2 heterostructure depend strongly on the biaxial strain. The absorption coefficient of this heterostructure is maximum in the far-ultraviolet region. We believe that with excellent optical properties as well as the ability to occur phase transitions due to strain engineering, the MoS_2/WS_2 heterostructure can become a potential material for applications in nanoelectronic and optoelectronic devices.

5 Acknowledgments

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Highlights

- MoS_2/WS_2 heterostructure is an indirect semiconductor with a type-II band alignment
- Semiconductor–metal transition can be found at large biaxial strain of 14%
- Effect of uniaxial strains on optical properties of heterostructure is quite small
- Optical parameters of MoS_2/WS_2 heterostructure depend strongly on the biaxial strain

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Competing Interests Statement

Manuscript Title: **Strain effects on the electronic and optical properties of Van der Waals heterostructure MoS$_2$/WS$_2$: A first-principles study**

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On behalf of co-authors

(x) I declare that I have no significant competing financial, professional, or personal interests that might have influenced the performance or presentation of the work described in this manuscript.

(x) I have described my potential competing financial, professional, and/or personal interests in the space below: (Provide details; use additional space if necessary.)

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