(a) 2-ZZ-WS₂-MoS₂-NR- r_z

(b) 4-ZZ-WS₂-MoS₂-NR- r_z

(c) 6-ZZ-WS₂-MoS₂-NR- r_z

(d) 8-ZZ-WS₂-MoS₂-NR- r_z

Size effect on the magnetic and electronic properties of the monolayer lateral hetero-structure WS₂-MoS₂ nanoribbon

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ABSTRACT

By using the VASP, we studied the magnetic and electronic properties of the monolayer lateral hetero-junction WS₂-MoS₂-nanoribbons (WS₂-MoS₂-NRs). Our results show that the NRs' edge chirality and width affect significantly its magnetic and electronic properties. The monolayer lateral hetero-junction ZZ-WS₂-MoS₂-NRs (ZZ: zigzag) exhibit metallic behavior and have considerable magnetic moment. Their magnetic moments decrease in the order of $N_z=2, 6$ and 4 (the width of NRs). While, the magnetic moment decreases with the increased r_z (the number of the Mo-S chains, $r_z \neq 0$ and $r_z \neq N_z$) at the same width N_z . The N_A -AC-WS₂-NR (AC: armchair) and N_A -AC-WS₂-MoS₂-NR-1 (the number of the Mo-S chain is 1) show metallic behavior when $N_A=3$ (the width of NRs). The other monolayer lateral hetero-junction AC-WS₂-MoS₂-NRs remain the nonmagnetic and semiconducting behavior as bulk. But they are indirect band-gap except for the $N_A=3$, $r_A=2$ (the number of the Mo-S chains) and $N_A=7$, $r_A=0$ when $N_A < 9$. However they are direct band-gap when $N_A \geq 9$. Their lowest and highest band gaps are 0.150eV and 0.581eV, respectively. These unique magnetic and electronic properties will provide guidance on the WS₂-MoS₂ hetero-junction application in nanodevice.

Keyword: Magnetic moment; Lateral hetero-structure; Nanoribbon; WS₂-MoS₂

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1. Introduction

The monolayer lateral heterojunction of the transition metal dichalcogenides (TMD) with unique mechanical, optical and electronic properties have a great potential application for new kinds of transistors [1], sensors [2], photodetectors [3], LEDs [4] and spin valleytronic devices [5]. The unique properties have motivated a lot of research interesting among science and engineering disciplines. For an example, the separation and recombination of photoinduced electron-hole pairs at a heterojunction interface are primary mechanisms governing the operation of solar cells, photodetectors and light-emitting devices [6]. In science scenario, first principles calculations play a very crucial role in. Especially, it is important to introduce a new material to experimentalists. The result from first principles calculations can be used to simplify an experimental recipe and reduce the experimental demands.

Both MoS_2 and WS_2 belong to the same family of the TMD. They have an indirect band gap in bulk, however they change to a direct band gap in monolayer type [7, 8]. Their lattice parameters are almost similar, which reminds us to study their electronic properties in the compound [9]. Since Li Q et al. [10] obtained the MoS_2 nanoribbons (NRs) by using an electrochemical method, many theoretical and experimental studies about the TMD NRs have been carried out [11-13]. Those studies showed both the MoS_2 and WS_2 NRs exhibited unusual magnetic and electronic properties. The ultra-narrow (less than 4nm) zigzag NRs have a magnetic ground state with electronic types ranging from metal, halfmetal, and even to semiconductor, whereas the armchair NRs was nonmagnetic and semiconducting [11-13]. The electronic and magnetic properties of the WS_2 and MoS_2 NRs are sensitive to the edge types and strains. For an example, the band gaps of armchair nanoribbons decrease with the increase of strain, and the magnetic moments of zigzag nanoribbons are strongly enhanced by strain [14, 15]. However, those properties can also be turned by applying an external electric field. For example, Dolui et al. showed that the band gap of armchair edge MoS_2 nanoribbon can be significantly reduced by applying an external transverse electric field, even leading to a metal-insulator transition beyond a certain critical field value [16]. Nevertheless, few

researchers considered the size effect on the properties of the WS₂ and MoS₂ NRs, not to mention the properties of the monolayer lateral heterojunction WS₂-MoS₂ NRs.

The lateral heterostructures WS₂-MoS₂ have been obtained by chemical vapor deposition (CVD) [17, 18]. According the experimental results, there are two kinds of the stability lateral heterojunction structures, which are zigzag (ZZ) and armchair (AC) edges, respectively. In this paper, we explored the unique magnetic and electronic properties of the monolayer lateral hetero-junction WS₂-MoS₂ NRs with the size effects by first-principles calculations. In the calculation, we change the chains rate between WS₂ and MoS₂ when total width keeps unchanged. For an example, the chains of MoS₂ (r_z) equals to 1, 2, and 3 if the chains of WS₂ equals to 3, 2 and 1 when total width $N_z=4$. Our results reveal that both their magnetic and electronic properties can be tuned precisely by controlling the edge type and the width of the monolayer lateral heterojunction WS₂-MoS₂ NRs. That could provide a new route of tuning the magnetic and electronic properties of WS₂-MoS₂ NRs and its derivatives for their promising applications in nanoelectronics and optoelectronics.

2. Models and Methods

In this work, we incorporate the projector augmented wave (PAW) scheme [19, 20] into the Vienna ab initio simulation package (VASP) [21]. Projector-augmented-wave (PAW) potentials were used to calculate electron-ion interactions. The generalized gradient approximation (GGA) [22] with the Perdew-Burke-Ernzerhof (PBE) functional [23] was used to the electron exchange correlation interactions. A vacuum layer of 18 Å is inserted in the perpendicular directions to avoid interaction between two supercells. The Monkhorst and Pack scheme of k point sampling is used for integration over the first Brillouin zone [24]. A 1×1×9 and 1×1×17 grids is used for k-point sampling for geometry optimization and calculations of density of states, respectively. A cutoff energy of 400eV is used in our NRs calculations. The equilibrium geometries were fully optimized. Both the lattice vectors and atom coordinates are relaxed with the tolerance of less than 0.02eV/Å

on each atom. The magnetic moments of the NRs are calculated both with and without spin polarization.

The quasi-one dimensional (Q1D) WS₂-MoS₂ NRs can be directly obtained by cutting a perfect WS₂-MoS₂ monolayer lateral hetero-junction along the zigzag (ZZ) or armchair (AC) direction. In order to obtain an available WS₂-MoS₂ monolayer lateral hetero-junction, we should choose its initial lattice constants before optimal calculation. For this purpose, infinite monolayer WS₂ and MoS₂ are first optimized to obtain their lattice constants. Then, we choose these constants as initial lattice constants of WS₂-MoS₂ monolayer lateral hetero-junction. The calculated W-S bond length, W-W and S-S (the distance of the S atoms on the top and bottom layers as show in the bottom panel of Fig. 2) distances are 2.42, 3.18, and 3.15 Å, respectively. These lengths are in agree well with the ones in Ref [15]. The lattice constant for the MoS₂ (a=3.183 Å) almost equals to the one of the WS₂ (a=3.182 Å). And Mo-S (d=2.413 Å) and W-S (d=2.417 Å) bonds are almost the same lengths. Therefore they can be matched perfectly in the monolayer lateral heterojunction as the experimental results [16]. The monolayer WS₂-MoS₂ lateral heterojunction is constructed based on 3.18Å lattice parameters. However, the monolayer WS₂ and MoS₂ have the different direct band gap as shown in Fig. 2 (a) and (b) respectively. The band gap 1.81eV of the WS₂ is slightly bigger than the 1.67eV of the MoS₂, which is in agreement well with the one in Ref. [15, 25].

Fig. 1. The energy band structure of the monolayer (a) WS₂ and (b) MoS₂.

According to Ref [14], the different WS₂-MoS₂ NRs should be constructed. There are only two

kinds of NRs, armchair and zigzag edges due to the symmetry of S at the edges, shown in Figs. 2. In Fig. 2, N_z (N_A) denotes to the total number of zigzag (armchair) Mo-S and W-S chains across the ribbon width, and r_z (r_A) is represented the number of zigzag (armchair) Mo-S chains in the N_z (N_A). Therefore, the zigzag (armchair) edge WS_2 - MoS_2 NRs can be denoted by N_z -ZZ- WS_2 - MoS_2 -NR- r_z (N_A -AC- WS_2 - MoS_2 -NR- r_A) as in Figs. 2a (Figs. 2b). When r_z (r_A)=0 or N_z (N_A), the NRs become the zigzag (armchair) edge WS_2 or MoS_2 NRs, respectively. For a comparison, all cases including zigzag (armchair) edge WS_2 and MoS_2 NRs are considered in this work.

Fig. 2. Atomic structure of the monolayer lateral heterojunction WS_2 - MoS_2 NRs: zigzag edge (a) and armchair edge (b). In (a) and (b), the upper and down views are shown on top (along y direction) and side panel (along z direction), respectively. The gray, pale purple and yellow balls respectively stand for W, Mo and S atoms. The unit cells are depicted by the black dashed lines. The width of zigzag edge and armchair edge NRs are depicted by red arrows, which are also described by red N_z and N_A , respectively. The number of Mo-S chains across the ribbon width are depicted by green arrows, which are also described by green r_z and r_A .

3. Results and Discussion

3.1 Size effects on magnetic properties of zigzag WS_2 - MoS_2 NRs

The calculated band structure of the N_z -ZZ- WS_2 - MoS_2 -NR- r_z ($N_z=2, 4, 6$ and 8) are shown in Figs. 3(a)-(d), and the Fermi level is always set to zero hereafter unless otherwise stated. From Fig. 3, we can see that there are several bands crossing the Fermi energy, so that each WS_2 - MoS_2 -NRs shows metallic behavior.

Furthermore, all the N_z -ZZ-WS₂-MoS₂-NR- r_z ($N_z=2, 4, 6$ and 8) NRs show magnetic properties except for 8-ZZ-WS₂-MoS₂-NR- r_z ($r_z=0$ and 8) due to the spin-splitting. The net spin density distribution (the scale is 0.001 e/B^3) on each atom of N_z -ZZ-WS₂-MoS₂-NR- r_z ($N_z=2, 4, 6$ and 8) are shown in Fig. 4(a)-(d). The magnetic moment as r_z for each N_z are presented in Fig. 4(e). Interestingly, for each 2-ZZ-WS₂-MoS₂-NR- r_z , the magnetic moment is mainly contributed by the S atoms at the **two edges** (left and right), seen in Fig. 4a. However, the magnetic moment is mainly contributed by the S atoms at the **right edge** for 4 and 6-ZZ-WS₂-MoS₂-NR- r_z , shown in Figs. 4b and 4c. Furthermore, the magnetic moment is mainly contributed by the Mo and W atoms at the two edges for 8-ZZ-WS₂-MoS₂-NR- r_z , presented in Fig. 4d. When $N_z=2, 4$ and 6 , the magnetic moments of W or Mo atoms at the edges are antiparallel to those of S atoms, shown in Figs. 4a-4c. However, for 8-ZZ-WS₂-MoS₂-NR- r_z ($r_z \neq 0$ and 8), the magnetic moments of W atoms are antiparallel to those of Mo atoms (magnetic moment of S atoms is antiparallel to that of Mo atoms), seen in Fig. 4d. For more clearly and quantificationally, we present magnetic moments as r_z for each N_z -ZZ-WS₂-MoS₂-NR, shown in Fig. 4e. When $r_z=0$ or N_z , the NRs just correspond to the zigzag edge WS₂ or MoS₂ NRs.

(c) 6-ZZ-WS₂-MoS₂-NR- r_z

(d) 8-ZZ-WS₂-MoS₂-NR- r_z

Fig. 3. The band structures of ZZ-WS₂-MoS₂-NRs that widths are $N_z=2, 4, 6$ and 8 . Here the black solid lines indicate the spin-up and the red dotted lines indicate the spin-down.

(a) 2-ZZ-WS₂-MoS₂-NR- r_z

(b) 4-ZZ-WS₂-MoS₂-NR- r_z

(c) 6-ZZ-WS₂-MoS₂-NR- r_z

(d) 8-ZZ-WS₂-MoS₂-NR- r_z

Fig. 4. The net spin density distribution (the scale is 0.001 e/B^3) on each atom of 2-ZZ-WS₂-MoS₂-NR- r_z (a), 4-ZZ-WS₂-MoS₂-NR- r_z (b), 6-ZZ-WS₂-MoS₂-NR- r_z (c), 8-ZZ-WS₂-MoS₂-NR- r_z (d), and the magnetic moment as r_z for each N_z -ZZ-WS₂-MoS₂-NR (e).

At first, we discuss the case of N_z -WS₂-NRs (or N_z -MoS₂-NRs). From Fig. 4(e), the magnetic

moment of 0.600 μ B (0.765 μ B) is the biggest for the WS₂-NRs (MoS₂-NRs) with zigzag edge when $N_z=2$. The magnetic moment of 0.549 μ B (0.528 μ B) when $N_z=6$ is slightly larger than the one of 0.507 μ B (0.524 μ B) when $N_z=4$. This result is due to the size effect. The value of 0.528 μ B for 6-ZZ-MoS₂-NRs is very close to the one of about 0.6 μ B in Ref [14]. When $N_z \geq 8$, the magnetic moments are equal to zero, which indicates the size effects limited to $N_z=8$ for the magnetic moment of N_z -WS₂-NRs (or N_z -MoS₂-NRs). Therefore we only considered the cases when $N_z \leq 8$.

For the NRs with the same width as the N_z -WS₂-NRs (or N_z -MoS₂-NRs), the magnetic moment is also affected by the hetero-structures interface structures. For 2-ZZ-WS₂-MoS₂-NR-1, the biggest magnetic moment is 0.768 μ B. While the magnetic moments are 0.514 μ B, 0.513 μ B and 0.502 μ B for 4-ZZ-WS₂-MoS₂-NR-1, 2 and 3, respectively. All of values decreases with the increased r_z (Mo-S chains number). The same tendency can be found for 6-ZZ-WS₂-MoS₂-NR-1(2), 3, 4 and 5, and their magnetic moments are 0.555 μ B, 0.551 μ B, 0.540 μ B and 0.503 μ B, respectively. Interestingly, although the magnetic moments of most cases are very weak for 8-ZZ-WS₂-MoS₂-NR- r_z ($r_z \neq 0$ and 8), the value of the 0.567 μ B ($r_z=1$ and $N_z=8$) is bigger than the one of the any case of the 4 and 6-ZZ-WS₂-MoS₂-NR- r_z ($r_z \neq 0$, 4 and 6). These phenomenons are mainly induced by the different hetero-structure interface structures.

3.2 Size effects on electronic properties of armchair WS₂-MoS₂ NRs

For keeping a consistency, the biggest width of calculated armchair NRs is limited to $N_A=11$ (18.4Å) according to the results of the size effects limited to $N_z=8$ (21.1Å) on the zigzag WS₂-MoS₂ NRs. The relationship between electronic structure and width of the N_A -AC-WS₂-MoS₂-NR- r_A is shown in Fig. 5. From Fig. 5a, there are bands crossing the Fermi energy when $r_A=0$ and 1, so that 3-AC-WS₂-NR and 3-AC-WS₂-MoS₂-NR-1 show metallic behavior. However, the other NRs are semiconducting and nonmagnetic, and they are indirect band-gap except for the 3-AC-WS₂-MoS₂-NR-2 and 7-AC-WS₂-MoS₂-NR-0 when $N_A < 9$. They show direct band-gaps at the Γ point from $N_A=9$, that are omitted for simplify. The band-gaps of the 3, 5, 7, 9 and 11-AC-WS₂-MoS₂-NR- r_A are listed in Table I. The band-gap as the width (N_A) of the MoS₂ NRs and

WS₂ NRs are shown in Fig. 6 (a). And the band-gap as the r_A are shown in Fig. 6 (b) when its width is a constant.

Fig. 5. The energy band structures of 3-AR-WS₂-MoS₂-NR- r_A (a), 5-AR-WS₂-MoS₂-NR- r_A (b) and 7-AR-WS₂-MoS₂-NR- r_A (c).

Fig. 6. The **band-gap (E (eV))** varies with the width of the MoS_2 NRs and WS_2 NRs (a), and varies as r_A (b) with different N_A .

Table I. The energy values **(the unit is eV)** of each band-gap from the 3 to 11-AR- WS_2 - MoS_2 -NR- r_A . The minimum and the maximum band-gaps are bold letter.

$r_A \backslash N_A$	3	5	7	9	11
0	-	0.453	0.380	0.419	0.509
1	-	0.485	0.367	0.421	0.496
2	0.150	0.495	0.385	0.456	0.516
3	0.306	0.485	0.398	0.453	0.493
4		0.490	0.407	0.458	0.496
5		0.523	0.415	0.469	0.498
6			0.457	0.474	0.503
7			0.451	0.462	0.521
8				0.511	0.519
9				0.527	0.507
10					0.581
11					0.579

From Table 1 and Fig. 6a, we can know that the WS_2 and MoS_2 NRs have the same change tendency as the width except for $N_A=3$. The minimum and the maximum band-gaps correspond to $N_A=3$ (5) and 11 for MoS_2 (WS_2) NRs, respectively. The band gap of the 11-AC- WS_2 NR (0.509eV)

is very close to the convergent value 0.5eV in Ref [15], and the band gap of the 11-AC-MoS₂ (0.579eV) is in agree well with 0.59eV in Ref [14]. From Fig. 6 (b) and Table I, we can know that the band gap is different when the chains rate is varied between WS₂ and MoS₂ for a constant width. In all the case, the lowest band gap is 0.150eV corresponding to the 3-AC-WS₂-MoS₂-NR-2 ($r_A=2$ and $N_A=3$) and the highest one is 0.581eV of the 11-AC-WS₂-MoS₂-NR-10 ($r_A=10$ and $N_A=11$). Thus, the optoelectronic and photovoltaic properties of AC-WS₂-MoS₂-NR can be tuned by changing the NR edge chirality and width.

From Fig. 5, we can know that 3-AC-WS₂-NR and 3-AC-WS₂-MoS₂-NR-1 are different from other armchair NRs. The key reason originates in the different atomic structures at the edges of these nanoribbons. The different atomic structures at edges induce the different band structures. To explain the difference, we plot Fig. 7 to show the atom structures at edges of these nanoribbons (3-AC-WS₂-MoS₂-NR- r_A ($r_A=0\sim3$)). In Fig. 7, we present the bond lengths of the neighbor atoms in the unite cell. From Fig. 7, the atom structure in Fig. 7 (b) is very different from the ones in Figs. 7 (a), (c) and (d). And the W-S (2.1624Å) and S-W (3.4971Å) bond lengths on the right side of the Fig. 7 (b) are the shortest and longest in all the bond lengths, respectively. This induces the W-S (2.1624Å) pair easily separated from the NR and the 3-AC-WS₂-MoS₂-NR-1 displaying metallic behavior. For the 3-AC-WS₂-NR in Fig. 7 (a), the average bond length 2.4037Å is bigger than the ones of 2.3853Å in Fig. 7 (c) and 2.3778Å in Fig. 7 (d). Furthermore, the electro-negativity of W atom is bigger than the Mo atom. These made the 3-AC-WS₂-NR showing metallic behavior. However, these phenomena will disappear as the width increase.

Fig. 7. The atom structure of the 3-AC-WS₂-MoS₂-NR- r_A ($r_A = 0 \sim 3$), respectively in (a)~(d), with the distance of the neighbouring atoms in the unite cell. The gray, pale purple and yellow balls respectively stand for W, Mo and S atoms.

The two-dimensional (2D) monolayer WS₂ and MoS₂ are semiconductors because of band gaps, shown in Fig. 1. The band gap originates in the periodicity of two dimensional systems. The monolayer ZZ-WS₂-NRs and ZZ-MoS₂-NRs exhibit metallic and magnetic properties, many of armchair NRs, such as AC-WS₂-NRs and AC-MoS₂-NRs are showing semiconducting properties. The main reason is due to their different boundary structure. There are two edges in each NR. The edge state induced by edges is dominant and very important when the nanoribbon is very narrow. For ZZ-NR, the edge states appear in the middle of the band gap and cross over band gap between conductance and valence bands, seen in Fig. 3. For AC-NRs, the edge states appear in the middle of the band gap, but not cross over band gap between conductance and valence bands, seen in Figs. 5 and 6. Furthermore, for each kind of NRs, the atomic structures at edge are affected by the width, which becomes more obvious as the size decrease. Thus, the monolayer zigzag NRs exhibit different magnetic properties, and the armchair NRs exhibit different band gaps.

4. Conclusions

By using the VASP, we study the size effects on the magnetic and electronic properties of the monolayer lateral hetero-junction WS₂-MoS₂-NRs with both zigzag and armchair edges in detail. The results are as follows:

- (1) The monolayer ZZ-WS₂-NRs and ZZ-MoS₂-NRs exhibit metallic and magnetic behavior, and

the magnetic moment decreases as following the order $N_z=2, 6$ and 4 . When $N_z \geq 8$, the magnetic moments are equal to zero, and the ZZ-WS₂-NRs and ZZ-MoS₂-NRs only exhibit the metallic behavior.

- (2) For the same width hetero-structure NRs with the ZZ-WS₂-NRs and ZZ-MoS₂-NRs, the magnetic moment is also affected by the hetero-structures interface structures. When $N_z=2, 4$ and 6 , the magnetic moments decrease with the increase of r_z ($r_z \neq 0$ and N_z), respectively.
- (3) The 3-AC-WS₂-NR and 3-AC-WS₂-MoS₂-NR-1 show metallic behavior. The other monolayer lateral hetero-junction AC-WS₂-MoS₂-NRs remain the nonmagnetic and semiconducting behavior as bulk. They are indirect band-gap except for the 3-AC-WS₂-MoS₂-NR-2 and 7-AC-WS₂-MoS₂-NR-0 when $N_A < 9$. And they show direct band-gaps when $N_A \geq 9$.
- (4) The WS₂ and MoS₂ NRs have the same change tendency as the width except for $N_A=3$. For the same width NRs, the band gap is different when the chains rate is varied between WS₂ and MoS₂. The lowest band gap is 0.150eV of 3-AC-WS₂-MoS₂-NR-2 while the highest one is 0.581eV of the 11-AC-WS₂-MoS₂-NR-10. Thus, the optoelectronic and photovoltaic properties of AC-WS₂-MoS₂-NR can be tuned by changing the hetero-structure NRs chirality and width.

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