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Tuning magnetism by strain and external electric field in zigzag Janus MoSSe nanoribbons

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ABSTRACT

Motivated by the successful synthesis of Janus monolayer MoSSe, we systematically study its zigzag nanoribbon (shorted as Z_n-JMoSSeNR) and investigate the electronic and magnetic properties modulated by the strain and external electric field. The pristine Z_7-JMOSSeNR structure is a ferromagnetic metal and possesses a magnetic moment of 0.99 μ_B/cell. Its spin density distribution covers on both edges. With the strain, a four-stage variation of magnetic moment occurs in the ribbon. The largest magnetic moment of 1.72 μ_B/cell is obtained under the strain of 14%. Under an external electric field, the magnetic moment decreases a little at first and then increases with the increase of the external electric field. The localization of spin density distribution could be modulated either by strain or electric field. Furthermore, with the combination of strain and external electric filed, an improved modulated response of the magnetic moment could be induced. Our investigations could help to design related spintronic nanodevices controlled by both strain and external electric filed.

1. Introduction

Two-dimensional (2D) monolayer transition metal dichalcogenide (TMD) can be easily mechanically exfoliated from bulk crystals due to their van der Waals (vdW) interactions between layers. Monolayer TMDs have attracted tremendous scientific and technological interests, due to its demonstrated remarkable mechanical, electronic and optical properties [1–18]. Besides monolayer TMDs, its one-dimensional (1D) nanoribbon structure, such as MoS_2 nanoribbon, has been considered as a promising 1D material for the next-generation nanoelectronic device [19]. The experimental and theoretical studies have been explored [20–32]. Similar to graphene nanoribbons [33–38], zigzag MoS_2 nanoribbons (Z-MoS_2NR) possess ferromagnetic metallic properties, while armchair ones have width-dependent semiconducting band gaps [31,32]. Their properties are also quite dependent on other factors, such as doping, defects, absorption, edges, strain and external electric field [20–32].

Janus monolayer MoSSe was successfully synthesized very recently [39]. The scientists first grew MoS_2 monolayer by chemical vapour deposition, then removed the top-layer sulfur atoms by hydrogen plasma and replaced the top-layer S atoms by hydrogen atoms, and last they used thermal selenization method to let Se atoms replace H atoms. Correspondingly, the top-layer S atoms were fully replaced by Se atoms. Such Janus monolayer MoSSe structure breaks the out-of-plane symmetry, leading to optical second harmonic generation and an intrinsic vertical piezoelectric response [39].

The charge of electron for the carry of information is only used in traditional electronics, which is limited for future applications. Spintronics [40], which can carry information by the usage of not only charge but also spin of electron, are considered as one of the next-generation innovations in science and technology. Great efforts are still needed to make breakthrough of magnetic materials, theoretical designs and predictions for future potential spintronic applications [40].

Motivated by the synthesis of Janus monolayer MoSSe and potential spintronic applications, zigzag Janus MoSSe nanoribbon, shorted as Z-JMoSSeNR, is tried to theoretically investigate here. Furthermore, the external modulation of electronic and magnetic properties could be essentially required for the future applications in the spintronic nanodevices. Since strain and external electronic field have been provided effective tuning of electronic and magnetic properties in zigzag graphene nanoribbons (ZGNRs) and Z-MoS_2NRs [25,27,34], in the present work, we perform a first-principle study of the modulated effects of strain and external electric field on electronic and magnetic properties and the combined

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modulations of two factors for a more precise control of the system.

2. Theoretical methods and models

The calculations are performed using density functional theory (DFT) implemented in SIESTA code [41]. Pseudopotentials with localized atomic-orbital basis sets are approached. The Ceperley–Alder (CA) [42] local spin density approximation (LSDA) and a double-ζ plus polarization basis sets are used. A plane-wave cutoff of 300 Ry is chosen during the calculations. To make all atomic positions fully relaxed, the force tolerance of 0.02 eV/Å is used. 1 × 41 × 1 Monkhorst-Pack k-point grid is used to sample Brillouin zone. To isolate the nanoribbons, a large spacing of at least 20 Å between ribbons is used to guarantee negligible interactions. The parameters used in DFT calculation for Janus monolayer MoSSe are in accordance with previous report [39].

According to the direction of terminations, the Janus monolayer MoSSe nanoribbons can also have two kinds of edges: armchair and zigzag ones, similar to graphene nanoribbons [33–35] and MoS_2 nanoribbons [26,31,43]. Based on previous works of TMDs, it is noted that armchair nanoribbons are nonmagnetic [26,31,43], and zigzag ones can exhibit magnetic properties [31,43]. Since we mainly focus on the magnetic properties in this work, the zigzag Janus MoSSe nanoribbons are chosen for the investigations. Similar to different types of edges in zigzag MoS_2 nanoribbons reported by the previous works, such as two edges terminate by S and Mo atoms [31,43], and the edges passivated by hydrogen atoms mainly with one-hydrogen passivated S atom and two-hydrogen passivated Mo atom [22,25,32], zigzag Janus MoSSe nanoribbons can also have these different edges. Different types of edges affect the electronic and magnetic properties in zigzag TMD nanoribbons [22,25,31,32,43]. Zigzag Janus MoSSe nanoribbons with Mo and S/Se edges have a larger edge reconstruction than hydrogen-passivated ones, and the former one also has a larger magnetic moment than the later one. According to previous hydrogen-passivated zigzag MoS_2 nanoribbons, which have one-H-passivated S edges and two-H-passivated Mo edges [22,25,32], in this work we study similar zigzag Janus MoSSe nanoribbons. Such kind of hydrogen passivation can keep coordination number of each atom as the same as the one in the bulk case and eliminate the dangling bond of bare Mo and S/Se edges.

Z-JMoSSeNRs are initially constructed from the cuts of monolayer Janus MoSSe. Similar to ZGNRs and Z-MoS_2NRs, Z-JMoSSeNRs are specified by the number of zigzag chains (n) along the ribbon and denoted as Z_n-JMoSSeNRs (Fig. 1(a)). To eliminate the dangling bonds, all the atoms at the edges are passivated by hydrogen atoms. Each Mo atom is passivated with two hydrogen atoms while each S or Se atom is passivated with one hydrogen atom. The external strain (see Fig. 1(a)) is simulated by variation the lattice constant along the ribbon's direction (y axis) as $\varepsilon = (a - a_0)/a_0$, where a and a_0 are the strained and the unstrained lattice constants, respectively. Under the stain condition, the lattice constant is fixed and all the atoms are fully relaxed. The external electric field is applied along x direction.

3. Results and discussion

3.1. Magnetic and electronic properties of Z-JMoSSeNR

In the present work, we study Z_7-JMoSSeNR as a representative model. In the fully relaxed nanoribbon structure, it can be seen that the distance between Mo and S (or Se) atom, $d_{Mo\text{-}S}$ (or $d_{Mo\text{-}Se}$), varies dependent on the position in the ribbon. In the Z_7-MoSSeNRs (Fig. 1), at the center of the nanoribbon, $d_{Mo\text{-}S}$ = 2.43 Å and $d_{Mo\text{-}Se}$ = 2.55 Å, while at the edge of the nanoribbon, the distances are enlarged to $d_{Mo\text{-}S}$ = 2.49 Å and $d_{Mo\text{-}Se}$ = 2.62 Å, originating from the edges' reconstructions.

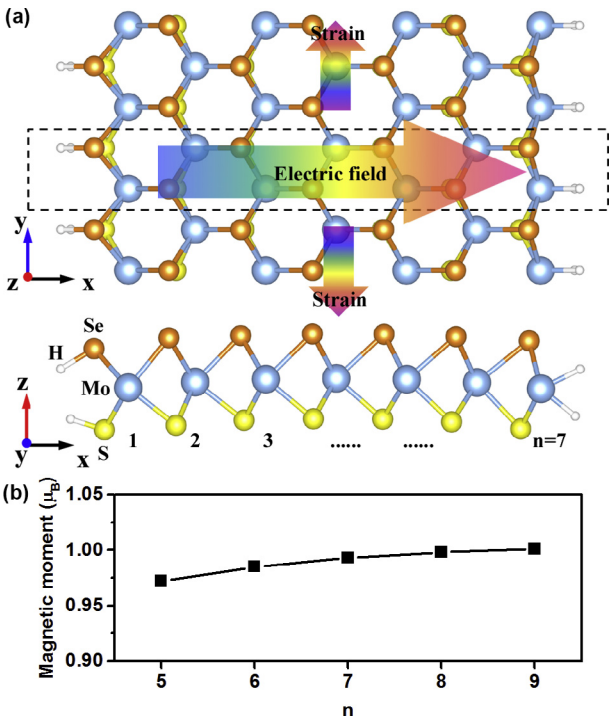

Fig. 1. (a) Top and side view of the structural model of zigzag Janus MoSSe nanoribbon. The nanoribbon with n zigzag chain (labelled by Mo atoms), is named as Z_n-JMoSSeNRs. The unit cell is indicated by a dashed rectangle. The strain is applied along the ribbon's direction (y axis). The external electric field is applied x direction. (b) Magnetic moments per unit cell for a series of Z_n-JMoSSeNRs (n = 5–9).

During the optimization of nanoribbons, both nonpolarized and spin-polarized computations are carried out to determine the ground state. It is found that the total energy of spin-polarized calculation is 25 meV/cell lower than that of nonpolarized one. Moreover, compared the ferromagnetic sate with the antiferromagnetic one, the total energy of the former is around 19 meV/cell lower than the later one. The total magnetic moment is around 0.99 μ_B/-cell, which is much larger than that of Z_7-MoS_2NRs (0.34 μ_B/cell) [25]. The magnetic moment per unit cell as a function of the ribbon's width is also plotted in Fig. 1(b). With the increase of the width, the magnetic moment slightly increases.

To understand the magnetic and electronic properties of Z_7-MoSSeNR, the spin-polarized band structure, density of states (DOS) and spin density distribution are calculated and shown in Fig. 2(a)–(c), respectively. In the electronic band structure, as there are two band lines (denoted as I and II) in the up-spin part and one band line (denoted as i) in the down-spin part crossing the Fermi level (E_F), it indicates that Z_7-MoSSeNR is a ferromagnetic metal. In the partial density of states (PDOS), it clearly shows that Mo atoms contribute the most crossing E_F. The spatial spin density distribution ($\rho_\uparrow$-$\rho_\downarrow$) also demonstrates that the unpaired electrons mainly localized on the Mo atoms, and 4d orbitals of Mo atoms contribute the most. As a comparison, the zigzag MoS_2 nanoribbon has a ferromagnetic order along the same edge but antiferromagnetic order along the opposite edge [25]. In the Janus MoSSe nanoribbon, as shown in Fig. 2(c), the unpaired electrons couple ferromagnetically at both edges, and Mo atoms at the edges have more contribution to the total spin moments, whereas the S and Se atoms at the edges contribute a small amount of spin. Thus