Tunable magnetic coupling in Mn-doped monolayer MoS₂ under lattice strain

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Abstract

First-principles calculations are conducted to study the electronic and magnetic states of Mn-doped monolayer MoS₂ under lattice strain. Mn-doped MoS₂ exhibits half-metallic and ferromagnetic (FM) characteristics in which the majority spin channel exhibits metallic features but there is a bandgap in the minority spin channel. The FM state and the total magnetic moment of 1 µB are always maintained for the larger supercells of monolayer MoS₂ with only one doped Mn, no matter under tensile or compressive strain. Furthermore, the FM state will be enhanced by the tensile strain if two Mo atoms are substituted by Mn atoms in the monolayer MoS₂. The magnetic moment increases up to 0.50 µB per unit cell at a tensile strain of 7%. However, the Mn-doped MoS₂ changes to metallic and antiferromagnetic under compressive strain. The spin polarization of Mn 3d orbitals disappears gradually with increasing compressive strain, and the superexchange interaction between Mn atoms increases gradually. The results suggest that the electronic and magnetic properties of Mn-doped monolayer MoS₂ can be effectively modulated by strain engineering providing insight into application to electronic and spintronic devices.

Keywords: monolayer MoS₂, Mn doping, magnetic exchange coupling, strain

(Some figures may appear in colour only in the online journal)

1. Introduction

After fabrication of graphene in 2004 [1], two-dimensional (2D) layered transition metal dichalcogenides (TMDCs) have been widely studied due to their unique electronic and magnetic properties as well as potential applications [2–8]. MoS₂ as an important member of TMDCs can be easily synthesized [6, 9, 10]. Monolayer MoS₂ has interesting electronic properties arising from quantum confinement effects [10, 11]. No magnetism has been found for most of the pristine 2D materials, such as, graphene, boron nitride sheets and monolayer MoS₂ but Zhao et al [12] found that substitutonal carbon doping in a honeycomb BN lattice favored spontaneous spin polarization and local magnetic moment. Thakur et al [13] reported that Mo doping induced magnetism in graphene through the energy shift at \( E_F \). Similarly, Zhou et al [14] observed that Mn, Fe, Co, Ni, Cu and Zn substitutions could induce magnetism in MoS₂ sheets. Pizzochero et al [15] predicted that Mo adatoms and antisites might induce local magnetic moments in monolayer 1T'-MoS₂. Zhang et al [16] demonstrated Mn dopant induced changes in electronic states of monolayer MoS₂. Komsa et al [17] found that Mo (S) adatoms, interstitials and Re dopants...
might lead to n-type doping and even magnetism in MoS$_2$, although S and Mo vacancies could not. Mathew et al. [18] demonstrated ferromagnetic behavior in 2 MeV proton-irradiated MoS$_2$ with a Curie temperature of 895 K, and ascribed the magnetization to the isolated vacancies, vacancy clusters, edges as well as lattice reconstruction. Lin et al. [19] summarized the defect behaviors in TMDs and deepened our understanding on the influences of defects on the physical and chemical properties. Ramasubramaniam et al. [20] discovered that substitutional Mn dopants in the range of 10%–15% might lead to ferromagnetism in monolayer MoS$_2$ at room-temperature. Qi et al. [21] found that the FM state of Mn-doped MoS$_2$ is highly stable and robust to the tensile strain. Roqueta et al. [22] observed the FM behavior in strained films and first-principles calculations demonstrated that tensile strain could enhance or even induce ferromagnetism in monolayers MX$_2$ (M = Sc, Ti, Zr, Hf, Ta, Cr; X = S, Se, Te) [23]. Commonly, monolayer NbS$_2$ and NbSe$_2$ exhibit nonmagnetic and metallic features, but they can be changed into a half metal with FM properties under tensile strain [24]. Li et al. [25] observed tunable magnetic exchange coupling and transformation from the FM to antiferromagnetic (AFM) states in Mn-silicene system under biaxial strain. Hence, doping and strain engineering are effective methods to modulate the magnetic properties of 2D materials [26–28] to broaden their applications in spintronics.

In this work, the coupling effects of lattice strain and Mn dopants on the electronic and magnetic states of MoS$_2$ are studied by first-principles calculations. If Mn is doped in MoS$_2$, the unit cell of MnS$_2$ characteristic of ferromagnetism with high Curie temperatures $T_C$ is generated [29]. The FM state is maintained and even enhanced under tensile strain, but transformed to the AFM state under compressive strain. The changes in the electronic states and magnetic coupling effects are analyzed and discussed.

2. Calculation details

First-principles calculations were carried out using MedeA-VASP [30–32] based on the plane-wave basis set by the projector-augmented wave method [33, 34]. The generalized gradient approximation of the Perdew–Burke–Ernzerhof [34–36] scheme was adopted to describe the exchange-correlation interactions. The valence-electron configurations of S, Mo, and Mn are $3s^23p^4$, $4d^55s^1$, and $3d^54s^2$, respectively and the kinetic energy cutoff for plane-wave expansion was set to 450 eV [37, 38]. A vacuum layer 1 Å thick was added perpendicular to the monolayer MoS$_2$ to avoid the interaction between adjacent layers. The Brillouin-zone integration was sampled using a $5 \times 5 \times 1$ k-mesh according to the Monkhorst–Pack scheme for structure relaxation and a $7 \times 7 \times 1$ k-mesh for single-point calculation. The structure was fully relaxed for an energy convergence of $1.0 \times 10^{-5}$ eV and force convergence of 0.01 eV Å$^{-1}$ [39, 40]. The in-plane biaxial strain was imposed by varying the lattice constant $a$ and is computed as $\varepsilon = (a - a_0) / a_0$, where $a_0$ and $a$ are the lattice constants of the monolayer MoS$_2$ in its equilibrium and strained states, respectively. Additionally, the DFT + U method with $U$ in the range of 1–5 eV is adopted for comparison. The $U$ parameters used in this work are referred to the values based on [20, 38, 41], and they were assigned to describe the correlation energy of doped Mn $3d$ states.

3. Results and discussion

Experimentally, hexagonal MoS$_2$ has the lattice parameter $a_0 = 3.16$ Å [42, 43]. After structural optimization, the lattice constant $a_0$ in monolayer MoS$_2$ is increased into 3.186 Å, which is in good agreement with the reported results [44–46]. In such a case, the equilibrium Mo–S bond length is about 2.413 Å, in reasonable agreement with the experimental/theoretical values of 2.41 Å [47–49]. Figure 1(a) plots the stress–strain curve of monolayer MoS$_2$ under biaxial tensile loading, the stress decreases sharply at a strain of 17%, characteristic of brittle fracture. As shown in the inset of figure 1(a), the Mo–S bond length is 2.570 Å at the strain of 17% and the Mo–S bonds will be broken after that strain. According to the DFT calculations, one of the Mo–S bond lengths in monolayer MoS$_2$ with only one Mo dopant 2.567 Å if a
tensile strain of 9% is applied. Hence, the biaxial strain in the range from \(-10\%\) to \(9\%\) is considered and it is still smaller than the intrinsic strain limit (~11%) [50, 51]. The \(2\times 2\), \(3\times 3\), \(4\times 4\), \(5\times 5\), and \(6\times 6\) supercells of Mn-doped MoS\(_2\) are adopted, in which one Mo atom is substituted by Mn atom, figure 1(b) shows the energy differences (\(\Delta E\)) between the spin-polarized and spin-unpolarized states. All the \(\Delta E\) values except that of \(2\times 2\) are negative, so the spin-polarized state is maintained for the larger supercells. Hence, the magnetism can be modified in monolayer MoS\(_2\) by atomic defects, which is similar to the results reported by [15–19].

Taking into account the valence electron configurations of Mo 4\(d^55s^1\) and Mn 3\(d^44s^2\), the electron will be introduced in the Mn-doped MoS\(_2\) resulting in n-type doping. Based on the DFT + \(U\) method, the DOS of Mn-doped MoS\(_2\) is calculated, and as an example, figure 2(a) shows the DOS of the \(5\times 5\times 1\) supercell, in which one Mo atom is substituted by Mn atom, corresponding to a doping concentration of 4%. The DOS changes a little with \(U\), but the Mn-doped MoS\(_2\) is always magnetic half-metal. Figure 2(b) shows the energy difference (\(\Delta E\)) between the spin-polarized and spin-unpolarized states as well as the magnetic moment in Mn-doped MoS\(_2\) as a function of \(U\). All the \(\Delta E\) values are negative, and the absolute value of \(\Delta E\) increases with \(U\) value, indicating that spin-polarized state is more stable for the larger \(U\) value. But the magnetic moment changes with \(U\) value little. No matter whether DFT or DFT + \(U\) is adopted, the system is in the FM state with 100% spin polarization, the minority spin channel displays an appreciable gap of 1.21 eV, but the DOS of majority spin channel is across the Fermi level. Hence, the \(U\) value affects the magnetic moment distribution and magnetic coupling in the Mn-doped MoS\(_2\) only a little. Accordingly, the DFT method is mainly adopted for the following calculations. Figure 2(c) shows the PDOS of Mn 3d orbitals and the second nearest Mo 4d orbitals and the nearest S 3p orbitals in Mn-doped MoS\(_2\). The states across the Fermi level are mainly from the Mn 3\(d\) and Mo 4\(d\) indicating the exchange interaction between them, which is similar to the double exchange interaction in Zener’s model [52, 53]. The \(d\) orbitals of Mn and Mo are located near the Fermi level in the majority spin channel. When the Fermi level is within the impurity band, double exchange usually dominates other exchange mechanisms. In fact, parallel or antiparallel coupling between Mn and Mo atoms via the neighboring S atom exists, as confirmed by the spin charge density in figure 2(d). Obviously, spin polarization takes place between Mn atom and its neighboring Mo/S atoms and the spin density is substantial at the doped Mn. The neighboring S atoms are antiferromagnetically coupled with the Mn dopant and the spin-polarized \(p\) orbitals of the S atoms are visible. The second nearest neighbor Mo atoms are ferromagnetically coupled with the doped Mn. That is, the exchange interaction between Mn and Mo takes place, resulting in a parallel coupling of localized spin through S atoms [52]. Figure 3 displays the magnetic moment and PDOS in \(6\times 6\), \(5\times 5\), \(4\times 4\) supercells of Mn-doped MoS\(_2\) under different strain. It is found that

![Figure 2.](image-url)

**Figure 2.** (a) DOS and (b) magnetic moment in \(5\times 5\times 1\) supercell of Mn-doped MoS\(_2\) as a function of \(U\), respectively. (c) The corresponding PDOS and (d) spin charge density using \(U = 0\), respectively.
the total magnetic moment is nearly 1 \( \mu_B \) and is almost independent on the supercell, no matter under a tensile or compressive strain. The strain enhanced hybridization between Mn 3\( d \) and Mo 4\( d \) orbitals is evidenced.

When two Mo atoms in the \( 5 \times 5 \times 1 \) supercell of monolayer MoS\(_2\) are substituted by Mn atoms, corresponding to a doping concentration of 8\%, three doping configurations are involved: (I) first-nearest neighboring, (II) second-nearest neighboring, (III) third-nearest neighboring. The formation energy of Mn-doped MoS\(_2\) of the three configurations is calculated as

\[
E_f = E_{\text{MoS}_2+\text{Mn}} - E_{\text{MoS}_2} - n\mu_{\text{Mn}} + n\mu_{\text{Mo}},
\]

in which \( E_{\text{MoS}_2+\text{Mn}} \) and \( E_{\text{MoS}_2} \) are the total system energies of the Mn-doped MoS\(_2\) and MoS\(_2\) after structural optimization, respectively. \( \mu_{\text{Mn}} \) and \( \mu_{\text{Mo}} \) are the chemical potential of one Mn and Mo atom, respectively. The calculated formation energies of the three doping configurations are \(-1.201\) eV, \(-0.304\) eV and \(1.763\) eV, respectively. The negative value indicates stable configuration, and the larger the absolute value is, the more stable is the configuration. So configuration (I) is the most stable one, and the energy difference \( \Delta E \) between the FM and AFM states is \(-1.055\) eV. The negative \( \Delta E \) indicates that configuration (I) exhibits FM state. The structural symmetry of the configuration (I) is reduced down to \( C_2 \) and the symmetry axis is highlighted by the dotted red line in figure 4(a). The Mn\(_1\)–Mo\(_1\) (\( l_1 \)) and Mn\(_2\)–Mo\(_1\) (\( l_2 \)) bond lengths are 3.183 Å and the Mn\(_1\)–Mn\(_2\) (\( l_3 \)) bond length is 3.241 Å (\( l_3 > l_1 = l_2 \)), which is similar to Jahn–Teller distortion [21]. The Mn and S atoms form a twisted triangular prism. As shown in figure 4(b), the S atoms near the doped Mn deviate from their original positions slightly. The Mn\(_1\)–S bond lengths are 2.391 Å, 2.354 Å, and 2.335 Å, respectively, and the Mn\(_2\)–S bond lengths are reduced by 1.07\%, 2.61\%, and 3.39\%, as compared with Mo–S bonds (2.417 Å). The formation energy of the configuration (I) is calculated by DFT + \( U \) method with different \( U \) values, and the results are listed in table 1. Apparently, the formation energy is increased with the \( U \) value, but the magnetic moment changes little. As shown in figure 4(c), the Mn-doped MoS\(_2\) is kept as magnetic half-metal, although the DOS changes with \( U \) value. So the FM state is still maintained if the DFT + \( U \) rather than DFT method is adopted. However, the DFT + \( U \) calculations consume more computing resources and the \( U \) values have little effects on the magnetic properties of Mn-doped MoS\(_2\).

Figure 5(a) shows the PDOS of Mn 3\( d \) orbitals, the second nearest Mo 4\( d \) orbitals and the nearest S 3\( p \) orbitals in the \( 5 \times 5 \times 1 \) supercell of MoS\(_2\) with two doped Mn. The doped Mn induces strong hybridization between the neighboring S/Mo atoms. In the energy range of \(-0.9\) eV to \(-0.55\) eV in the majority spin channel, there are states from two Mn 3\( d \) orbitals. Due to the unpaired electrons in Mn 3\( d \)

\[ \text{Figure 3. (a) Magnetic moment in (a) } 6 \times 6 \times 1 \text{ (b) } 5 \times 5 \times 1 \text{ and (c) } 4 \times 4 \times 1 \text{ supercells of Mn-doped MoS}_2 \text{ as a function of strain, (d)-(f) the PDOS under a strain of } -7\%, \text{ and (g)-(i) the PDOS under a strain of } 5\%, \text{ respectively.} \]
Figure 4. (a) Relaxed structure of Mn-doped MoS$_2$ in the $5 \times 5 \times 1$ supercell with a doping concentration of 8% with the red dotted line indicating the symmetry axis, (b) top view structure of the supercell in (a), (c) the corresponding DOS as a function of $U$.

Table 1. Formation energies and magnetic moments of the configuration (I) calculated using different $U$ values.

<table>
<thead>
<tr>
<th>$U$ (eV)</th>
<th>1.5</th>
<th>2</th>
<th>2.5</th>
<th>3</th>
<th>3.5</th>
<th>4</th>
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</thead>
<tbody>
<tr>
<td>Formation energy (eV)</td>
<td>$-1.924$</td>
<td>$-1.101$</td>
<td>$-0.257$</td>
<td>1.085</td>
<td>1.339</td>
<td>2.139</td>
</tr>
<tr>
<td>Magnetic moment ($\mu_B$)</td>
<td>2</td>
<td>2</td>
<td>2</td>
<td>2.01</td>
<td>2.08</td>
<td>2.33</td>
</tr>
</tbody>
</table>

Figure 5. The PDOS (a) of Mn-doped MoS$_2$ in the $5 \times 5 \times 1$ supercell, (b) of Mn$_1$ and (c) of Mn$_2$, respectively, (d) spin charge density of Mn-doped MoS$_2$ in the $5 \times 5 \times 1$ supercell, in which dark gray and cyan represent positive and negative spin densities (0.003 e Å$^{-3}$), respectively.
weakened, but that above the Fermi level (in the energy range of 0.1 eV–0.5 eV) is enhanced. As the tensile strain increases, the Mn-doped MoS2 always maintains half-metal characteristics, but the bandgap in the minority spin channel is reduced gradually. Figure 7(d) displays electron transfer of Mn1, Mn2, S3, Mo1, Mo5 (labeled in figure 4(a)). As the tensile strain increases, more electrons are lost from the Mo1, Mo5, Mn1 and Mn2 atoms, but the S3 atom gains more electrons. At the tensile strain of 7%, the excess charge on S3 and the electron depletion on Mn1, Mn2, Mo1, and Mo5 are 0.542, 0.979, 0.982, 1.229, and 1.231 e, respectively. The excess charge on S3 is increased by 11% at a tensile strain of 7%, and electron depletion on Mn1, Mn2, Mo1, and Mo5 is enhanced by 33%, 32%, 4%, and 5%, respectively. Therefore, Mn atoms have stronger interactions with neighboring S and Mo atoms under tensile strain resulting in stronger ferromagnetism.

The binding energies of the Mn-doped MoS2 under compressive strain are shown in figure 8(a). The binding energy remains positive under compressive strain, indicating a stable doping configuration and the binding energy is gradually reduced with increasing compressive strain. Figure 8(b) displays the distances between the Mn1 atom and its neighboring Mo atoms and the bond lengths between Mn1 and its nearest S atoms. They decrease with the increasing compressive strain almost linearly, but sharply increase at a compressive strain of 7%. This can be ascribed to the slightly out-of-plane displacement of Mn/S atoms. The bond length between the Mn2 atom and its neighboring S/ Mo atoms changes in the same trend. Figure 8(c) describes the exchange energy ($E_{ex}$) between the FM and AFM states of the Mn-doped MoS2. As the compressive strain increases, the absolute values of the $E_{ex}$ decreases, indicating lower stability of FM. The Curie temperature $T_C$ also decreases as reported in [57]. When the compressive strain is smaller than 7%, the ground state of the Mn-doped MoS2 is the FM state due to the double-exchange interaction. At the compressive strain of 7%, the Mn-doped MoS2 transforms from the FM to AFM states because of the superexchange interaction between two Mn dopants. At a compressive strain larger than 7%, small buckles are induced on the Mn-doped MoS2 and the two Mn dopants cooperate through the super-exchange interaction via the middle S atoms and the AFM state is more favorable as confirmed by the positive exchange energy $E_{ex}$. The compressive strain induced FM to AFM transformation was reported previously [25]. As shown in figure 8(d), the magnetic moment of Mn-doped MoS2 and two Mn dopants decreases with the compressive strain gradually and becomes zero at a compressive strain of 7%. The spin density of Mn-doped MoS2 under a compressive strain of 3% is shown in the inset of figure 8(d). The neighboring S atoms are antiferromagnetically coupled with the Mn dopants and the spin density is contributed by the Mn dopant. The calculated magnetic moment of the Mn1, Mn2, Mo1 and

Figure 7. PDOS of Mn-doped MoS2 under a tensile strain of (a) 1%, (b) 4% and (c) 7%; (d) electron transfer. The Fermi level is set to zero.
S3 atoms (as marked in figure 4(a)) at the compressive strain of 3% is 0.998, 0.997, −0.093, and −0.031 μB, respectively.

Figure 9 shows the PDOS of Mn-doped MoS2 under compressive strain and apparently, the density of states of Mn, the nearest neighboring S and the nearest neighboring Mo atoms are redistributed. At a strain of 3%, the defect states from the hybridization between Mn 3d and S 3p orbitals are below the Fermi level in the energy range of −0.9 eV to −0.5 eV in the majority spin channel (figure 9(a)), and there are states across the Fermi level in the majority spin channel, which is mainly from the Mn 3d and Mo 4d orbitals. In the minority spin channel, there are unoccupied states from the Mn 3d orbitals in the energy range of 0.05 eV–0.15 eV above the Fermi level. The Mn-doped MoS2 still exhibits half-metal characteristics. When the compressive strain is increased to 6%, the occupied states from hybridization between the Mn 3d and S 3p orbitals are in the energy range of −0.7 eV to −0.3 eV in the majority spin channel (figure 9(b)), and the states across the Fermi level in the minority spin channel are lowered as a result of enhanced delocalization of Mn 3d and Mo 4d orbitals. Meanwhile, the states of Mn 3d orbitals shift across the Fermi level in the minority spin channel and the Mn-doped MoS2 changes from half-metallic to metallic. The states of both the minority and majority spin channels move to the Fermi level with increasing compressive strain. The spin splitting of Mn 3d orbitals is gradually reduced (figures 9(a) and (b)) as well as the magnetic moments of the Mn-doped MoS2. At the compressive strain of 7%, the PDOS of the majority and minority spin channels are symmetric with each other (figure 9(c)) and the total magnetic moment becomes zero. Furthermore, the states of the Mn 3d orbitals become more localized in the energy range of −0.48 eV to −0.08 eV below the Fermi level. The hybridization between Mn and Mo atoms becomes very weak at the compressive strain of 7%, and the superexchange interaction between Mn atoms becomes stronger and even exceeds that between Mn and Mo atoms. Figure 9(d) displays the PDOS of the Mn1 and Mn2 3d orbitals at a compressive strain of 7%. The PDOS of the minority and majority spin channels are symmetric. The exchange splitting of Mn 3d orbitals is reduced down to zero, but the crystal-field splitting still exists. The states near the Fermi level are contributed by Mn1 dz², x² − y² and Mn2 dz², xy, indicating the strong interaction between two Mn atoms. Strong hybridization between Mn1 and Mn2 atoms in the energy range of −0.4 eV–0.3 eV is evidenced. The electron transfer of Mn1, Mn2, S3, Mo1, and Mo5 (labeled in figure 4(a)) has been calculated based on Bader analysis. The excess charge on S3 and the depletion of electrons on Mn1, Mn2, Mo1, and Mn5 are 0.483, 0.654, 0.664, 1.182 and 1.173 e, respectively, at zero strain. As the compressive strain increases, electron depletion in the Mo1/Mo5 atoms is reduced, but more electrons are depleted from the Mn1/Mn2 atoms. The interaction between Mo and S atoms is weakened, but the interaction between Mn and S atoms is enhanced. At a compressive strain of 7%, the excess
charge on $S_3$ and electron depletion on $Mn_1$, $Mn_2$, $Mo_1$, and $Mo_5$ are 0.433, 0.796, 0.798, 1.132 and 1.109 e, respectively, and the stronger interaction between Mn dopants results in the stronger anti-ferromagnetism.

4. Conclusion

The electronic states and magnetic properties of Mn-doped monolayer MoS$_2$ are studied based on first-principles calculations. The magnetic properties and Curie temperature ($T_C$) of the Mn-doped MoS$_2$ can be tuned by lattice straining. At zero strain, the Mn-doped MoS$_2$ is FM with $T_C$ above the room temperature. As for the monolayer MoS$_2$ with a small doping concentration, the FM state is maintained under both tensile and compressive strain. If the doping concentration is substantially increased, FM and $T_C$ will be improved remarkably under tensile strain. As the tensile strain increases, the stability of FM is enhanced because of increased covalent bonding between the Mn and S atoms and charge redistribution in the Mn 3$d$ orbitals. However, spin polarization in the Mn 3$d$ orbitals is reduced with increasing compressive strain and the Mn-doped MoS$_2$ is changed from the half-metallic FM state into metallic AFM state at a compressive strain of 7%. The strong FM order with high $T_C$ suggests potential applications in spintronic devices.

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