Strain robust spin gapless semiconductors/half-metals in transition metal embedded MoSe$_2$ monolayer

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Abstract
The realization of spin gapless semiconductor (SGS) and half-metal (HM) behavior in two-dimensional (2D) transition metal (TM) dichalcogenides is highly desirable for their applications in spintronic devices. Here, using density functional theory calculations, we demonstrate that Fe, Co, Ni substitutional impurities can not only induce magnetism in MoSe$_2$ monolayer, but also convert the semiconducting MoSe$_2$ to SGS/HM system. We also study the effects of mechanical strain on the electronic and magnetic properties of the doped monolayer. We show that for all TM impurities we considered, the system exhibits the robust SGS/HM behavior regardless of biaxial strain values. Moreover, it is found that the magnetic properties of TM–MoSe$_2$ can effectively be tuned under biaxial strain by controlling the spin polarization of the 3$d$ orbitals of Fe, Co, Ni atoms. Our findings offer a new route to designing the SGS/HM properties and modulating magnetic characteristics of the TM–MoSe$_2$ system and may also facilitate the implementation of SGS/HM behavior and realization of spintronic devices based on other 2D materials.

Keywords: transition metal dichalcogenides, spin gapless semiconductor, half-metals, strain engineering

Supplementary material for this article is available online

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

To improve the performance of spintronic devices, materials with high spin polarization are highly desired [1–3]. Spin gapless semiconductor (SGS), first proposed by Wang [4], not only have the full spin polarized electrons and holes, but also have no gap in the electronic spectrum, that is no energy is required to excite electrons from the valence band to the conduction band. Half-metallic (HM), which are metallic in one spin channel and semiconducting in the other spin channel, can achieve complete spin polarization at the Fermi level [5–7]. Due to 100% spin-polarization of the carriers at the Fermi level, SGS and HM materials have been considered as the most promising candidates for applications in spintronics. Therefore, great effort has been devoted to search for SGS and HM materials. Previous studies demonstrated that SGS and HM have been found in a large number of systems, including transition-metal oxides, transition-metal chalcogenides, perovskites, and Heusler compounds [8–10].

Interestingly, SGS and HM behaviors have also been predicted in two-dimensional (2D) materials, such as graphene, transition metal carbides and nitrides (also known as MXenes), and black phosphorus by introducing impurities [11–13], creating defects, [14, 15], and applying strain [16, 17]. Our previous works indicated that gold-embedded zigzag graphene nanoribbons (ZGNRs) can be SGS [18], and Pt-embedded ZGNRs exhibit a semiconductor—metal—HM transition as the position of Pt substitutional impurities in the ribbon changes from the center to edge sites [19]. Yafei Li et al reported the SGS—metal—HM transition in N-doped ZGNRs [11]. The HM behavior was also found in Re doped armchair MoSe$_2$ nanoribbon [20]. Fe doped MoSe$_2$ and Mn, Fe, Co, Ni doped WS$_2$ [21, 22]. In addition to impurities introduction, strain engineering is also an effective approach to tune electronic and magnetic properties of 2D materials [23–25]. For instance, strain generated by wrinkles can induce magnetism and modulate the optical band gap of ReSe$_2$ [26]. It was predicted that band gap of zigzag BN nanoribbons can be obviously decreased as tensile strain increases [27]. The deformation in monolayer black phosphorus can significantly tune the band gap and induce a transition from semiconductor to metal [28]. Likewise, a direct-to-indirect band gap and a semiconductor-to-metal transition can be caused by mechanical strain in transition metal dichalcogenides (TMDs) [29]. Under a biaxial strain, HM and SGS can be observed in monolayer MXenes [16]. The tensile strain can significantly enhance the magnetic moments and gives rise to a half-metallic character in NbS$_2$ and NbSe$_2$ [30]. By applying strain, the half-fluorinated BN and GaN sheets exhibit intriguing magnetic transitions from ferromagnetism to antiferromagnetism, and a half-metallic behavior can be achieved in the layers under a compressive strain of 6% [31]. In Al-doped MoSe$_2$ monolayer, magnetism was reported to disappear under compressive strain, while the magnetism is preserved under tensile strain [32]. The Co-doped WSe$_2$ monolayer can be transformed from magnetic semiconductor to half-metallic material under strain, as the first-principles calculation indicate [33]. The above results indicate that the electronic and magnetic properties of 2D materials are sensitive to the presence of dopants and external strain, so that it is meaningful to search for SGS and HM behavior in such systems.

TMDs, a class of inorganic 2D materials, have attracted much attention in recent years due to their intriguing electronic, optical and chemical properties [34–36]. MoSe$_2$ monolayer, one of the most studied members of the TMD family, has been successfully fabricated by mechanical exfoliation, chemical vapor deposition (CVD) and molecular beam epitaxy (MBE) [37–41]. Benefiting from the direct band gap of 1.44 eV [42, 43] and high carrier mobility [44], MoSe$_2$ monolayer shows good potentials for applications in various electronic devices including field effect transistors (FET) [45, 46], photodetectors [47] and phototransistors [48].

However, there are few reports on SGS or HM in MoSe$_2$ monolayer to date. In this work, by means of systematic density functional theory (DFT) calculations, we explore the electronic and magnetic properties of MoSe$_2$ with transition metal (TM) atoms (Fe, Co, Ni) embedded into the atomic network in substitutional positions (TM–MoSe$_2$). The results reveal that Fe/Ni–MoSe$_2$ system shows the HM, while Co–MoSe$_2$ exhibits the SGS behavior. Moreover, the SGS/HM is robust in TM–MoSe$_2$ independent of the magnitude of biaxial strain. In contrast, the biaxial strain can effectively modulate the magnetic properties of TM–MoSe$_2$ by controlling the
Figure 3. Spin-densities of (a) Fe–, (b) Co– and (c) Ni–MoSe2. The isosurface is set to be 0.004 e/Å³. The red regions represent spin-up density.

spin polarization of TM-3d orbitals. These results suggest that strain engineering is an effective route to achieve SGS/HM behavior and tune the magnetic properties in TM–MoSe2.

2. Computational methods

Our calculations were carried out using the Vienna *ab initio* simulation package (VASP) [49, 50] based on DFT. The generalized gradient approximation (GGA) with the Perdew–Burke–Ernzerhof (PBE) [51] parametrization was employed to deal with the exchange-correlation functional. We also tested on-site Coulomb interaction using PBE + U functional [52] to confirm our results. The values of Hubbard term $U$ are 3.5, 2.8 and 3.4 eV for Fe, Co and Ni atoms, respectively [53]. The projector-augmented-wave (PAW) method was used to describe electron-ion interactions [54].

The energy cutoff of the plane wave basis was set to 500 eV. The convergence criterion of the total energy and force were $10^{-6}$ eV/atom and 0.01 eV Å⁻¹, respectively. A $k$-point sampling of $11 \times 11 \times 1$ was used for geometry optimizations and self-consistent calculations, and a vacuum region of 15 Å was introduced to avoid interaction between periodic images of the slabs.

3. Results and discussion

Prior to modeling the substitution of Fe, Co, Ni atoms in MoSe2 monolayer, we first checked the accuracy of our approach by evaluating the lattice constant of pristine MoSe2. We found that the optimized lattice constant of MoSe2 monolayer is 3.32 Å, in good agreement with the experimental data [38] and previous theoretical reports [55, 56]. The PBE + $U$ functional also gives the same lattice constant (see table S1) (http://stacks.iop.org/JPCM/32/365305/mmedia).

Doping can be modeled in a $4 \times 4$ MoSe2 supercell by substituting a Mo or Se atom for Fe, Co or Ni atoms, respectively. The atomic models illustrating the substitutional dopants in the Mo and Se sites in MoSe2 monolayer are shown in figure 1. When Fe, Co, Ni atoms are embedded into the Mo site of MoSe2, the atoms form six covalent bonds with the nearest Se atoms. The bond lengths of TM–Se are 2.41 Å, smaller than that of Mo–Se (2.54 Å). When TM atoms are embedded at the Se site, three covalent bonds are formed between the TM atom and the nearest Mo atoms. TM–Mo bond lengths are 2.39 Å, 2.44 Å and 2.51 Å, respectively.

Figure 4. Band structures and the corresponding charge densities of the bands (indicated by the red and blue dashed lines) near the Fermi level for (a) Fe–, (b) Co– and (c) Ni–MoSe2. The red and blue solid lines indicate spin-up and spin-down channels in the band structures, respectively. The position of the Fermi level is indicated by the black dashed lines. The red and blue regions refer to the spin-up and spin-down states, respectively. The isosurface is set to be 0.004 e/Å³.

To assess the energetics and stability of the system with Fe, Co and Ni atoms embedded in MoSe2, we calculated the formation energy of Fe, Co and Ni atoms at different sites of
Figure 5. (a) PDOS of pristine MoSe$_2$. PDOS of (b) Fe–, (b) Co– and (c) Ni–MoSe$_2$. The black dashed lines indicate the positions of the Fermi level. The positive and negative values represent spin-up and spin-down channels, respectively.

Figure 6. Magnetic moments and electronic characteristics of Fe–, Co– and Ni–MoSe$_2$ under biaxial strain.

MoSe$_2$ monolayer. The formation energy $E_f$ is defined as $E_f = E_{TM@Mo/Se} + \mu_{Mo/Se} - \mu_{TM} - E_{MoSe_2}$, where $E_{TM@Mo/Se}$ and $E_{MoSe_2}$ are the total energy of TM–MoSe$_2$ and pristine MoSe$_2$ respectively, and $\mu_{TM}$ is the chemical potential of TM atom in the isolated TM dimer ($\mu_{TM} = \frac{1}{2}E_{TM2}$). We chose dimer as the reference system to assess the stability of the substitutional configurations with regard to clustering on the surface, with the dimer being the smallest cluster. $\mu_{Mo/Se}$ is the chemical potential of Mo/Se atom, which depends on the experimental situation. Here, we assume that $\mu_{Mo}$ and $\mu_{Se}$ are in a thermal equilibrium with MoSe$_2$, so that $\mu_{Mo} + 2\mu_{Se} = E_{MoSe_2}$ [57, 58]. For the Mo-rich condition, $\mu_{Mo}$ is calculated from the bulk Mo structure ($\mu_{Mo}^{\text{Mo-rich}} = \mu_{Mo\text{, bulk}}$), $\mu_{Se}$ is taken as $\mu_{Se}^{\text{Mo-rich}} = \frac{1}{2}(E_{MoSe_2} - \mu_{Mo\text{, bulk}})$ and defined as 0 eV. Analogously, for the Se-rich condition, $\mu_{Se}$ is determined from the Se$_2$ dimer ($\mu_{Se}^{\text{Se-rich}} = \frac{1}{2}/E_{Se_2}$), $\mu_{Mo}$ is calculated as $\mu_{Mo}^{\text{Se-rich}} = E_{MoSe_2} - 2\mu_{Se\text{, Se}_2}$. According to the above definition, a more negative $E_f$ value indicates a higher stability of the TM–MoSe$_2$. The calculated values of formation energy are presented in figure 2. It is evident that the TM@Mo configurations are energetically more favorable under the Se-rich condition, which is consistent with the recent reports [21, 59]. $E_f$ values exhibit a following trend: $E_f$(Fe) ($-4.34$ eV) $< E_f$(Co) ($-3.67$ eV) $< E_f$(Ni) ($-2.51$ eV) in the Se-rich limit, indicating that the Fe@Mo system is more energetically favorable than the others. We performed test calculations of the formation energy using the PBE+$U$ functional, and found that the trend of $E_f$(Fe) ($-3.35$ eV) $< E_f$(Co) ($-3.22$ eV) $< E_f$(Ni) ($-2.39$ eV) is the same in the Se-rich limit (see table S1). Different from the TM@Mo case, the TM@Se configurations are more favorable under the Mo-rich condition. However, as TM impurities at the Mo positions are energetically more favorable in a wider range of Se chemical potential, we focus on the electronic and magnetic properties of MoSe$_2$ monolayer with the former.

In order to get insight into the magnetic properties of TM–MoSe$_2$, the spin-densities in these systems are shown in figure 3. It can be seen that the spin densities are mainly localized on TM atoms and the neighboring Mo atoms. The local magnetic moments of TM atoms exhibit a trend of $M_{Se}$ (0.25 $\mu_B$) $< M_{Co}$ (0.88 $\mu_B$) $< M_{Fe}$ (1.38 $\mu_B$). The neighboring Mo atoms have the magnetic moments of 0.11, 0.22 and 0.19 $\mu_B$ in Fe–, Co– and Ni–MoSe$_2$, respectively. For Fe–MoSe$_2$, the total magnetic moment is 2.00 $\mu_B$, mostly coming from
the Fe atom and partly from its neighboring Mo atoms. The total magnetic moments of Co–MoSe₂ and Ni–MoSe₂ are 2.67 and 1.89 μB, which mainly stem from the neighboring Mo atoms and partly from Co/Ni atoms. The PBE + U calculations were also performed. The total magnetic moments of Fe–MoSe₂, Co–MoSe₂ and Ni–MoSe₂ are 2.00, 2.75, 1.86 μB with PBE + U method, respectively. There are no noticeable changes for magnetic moments of TM–MoSe₂ (see table S1), which confirmed the reliability of our results.

To investigate the effects of TM impurities on the electronic properties of MoSe₂ monolayer, the spin-polarized band structures were calculated and presented in figure 4. At the PBE level of theory, the pristine MoSe₂ exhibits a direct band gap of 1.44 eV, which agrees well with previously reported values [55, 56]. After TM atom introduction, flat impurity states can be clearly observed in the band gap of MoSe₂. For Fe–MoSe₂, it is evident from figure 4(a) that the spin-up channel is metallic with a band crossing the Fermi level, while the spin-down channel remains semiconducting with a gap of 0.91 eV. Therefore, Fe–MoSe₂ presents HM character and can provide 100% spin-polarized current. Co–MoSe₂ exhibits a semiconducting character with a band gap of 0.42 and 0.75 eV for the spin-up and spin-down channels, respectively, as indicated in figure 4(b). Interestingly, the valence band maximum (VBM) of the spin-up channel and the conduction band minimum (CBM) of the spin-down channel are both at the K point, and the band gap is 0.06 eV. According to Wang and Hu [4, 18], the band gap of approximately 0.1 eV or less than 0.1 eV can be defined as ‘gapless’. Thus, the band structure can be assumed to be gapless, which means that Co–MoSe₂ shows an SGS behavior. As for Ni–MoSe₂, the spin-up channel is semiconducting with a gap of 0.21 eV, while the spin-down VBM crosses the Fermi level and displays metallicity (see figure 4(c)). Thus, Ni–MoSe₂ is also HM, similar to the case of Fe–MoSe₂. The corresponding charge densities of the bands near the Fermi level (indicated by the red and blue dashed lines) are presented in the right panel of figure 4, which indicates that the spin-up and spin-down states near the Fermi level mainly come from TM atoms and the neighboring Mo atoms in all cases.

Next, to gain a deeper understanding of the changes in the electronic structure for TM–MoSe₂, we also calculated the projected density of states (PDOS), which are presented in figure 5. In the pristine MoSe₂ monolayer, the CBM is mainly dominated by the Mo dₓ² orbitals, while the VBM is mostly described by the Mo dₓᵧ + dₓ² orbitals (figure 5(a)), consistent with the previously obtained results [55, 56]. Upon embedding TM atoms, it is clear from figure 5 that the bands near the Fermi level are spin polarized. Specifically, for Fe–MoSe₂, two PDOS peaks were observed near the Fermi level for the spin-up channel, which are dominated by the Fe dₓᵧ + dᵧ² and Mo dₓ² orbitals, as illustrated in figure 5(b), while the spin-down channel remains semiconducting. Thus, Fe–MoSe₂ is HM with 100% spin-polarized current near the Fermi level. For Co–MoSe₂, Co atom induces impurity states in the energy range of −0.5 to 0.5 eV. The spin-up impurity states near the Fermi level are mainly composed of the Co dₓᵧ + dᵧ² and Mo dₓ² orbitals, while the spin-down impurity states near the Fermi level are dominated by the dₓ² orbitals of Co and Mo atoms. In Ni–MoSe₂, the spin-up channel is still semiconducting, whereas the spin-down channel is gapless, with the states mainly contributed by the Ni dₓᵧ + dᵧ², dₓ² and Mo dₓ² orbitals. Therefore, Ni–MoSe₂ shows half-metallicity, similar to the case of Fe–MoSe₂. These results indicate that SGS and HM can be obtained in the MoSe₂ monolayer by introducing Fe, Co and Ni atoms.
Figure 8. Band structures of (a) Fe–, (b) Co– and (c) Ni–MoSe$_2$ under $-5\%$, $0\%$ and $5\%$ biaxial strain, respectively. The red and blue solid lines indicate spin-up and spin-down channels in the band structures, respectively. The Fermi level position is indicated by the black dashed lines.

Previous studies suggested that the external strain can play an important role in practical applications of 2D materials, as it can effectively tune the electronic and magnetic properties of various 2D systems, such as graphene, MoS$_2$, BN and GaN [27–31]. We also studied the effects of strain on TM-embedded MoSe$_2$. The biaxial strain was defined as $\varepsilon = \Delta c/c_0$, where the unstrained and strained lattice constants of TM–MoSe$_2$ are $c_0$ and $c = c_0 \pm \Delta c$, respectively. The tensile or compression strain was modeled by first increasing lattice constant $c$, then reoptimizing the atomic structure with the elongated lattice constant kept fixed. We investigated the strain dependence of the magnetic moment in TM–MoSe$_2$ by varying the strain from $-5\%$ to $5\%$, as shown in figure 6. It can be seen that the variation of magnetic moments with strain is drastically different for the Fe–MoSe$_2$, Co–MoSe$_2$ and Ni–MoSe$_2$ systems. For the Fe–MoSe$_2$, the magnetic moment is $2 \mu_B$ for strain values from $-4\%$ to $5\%$, which is due to that the spin polarization of the Fe 3$d$ orbital near the Fermi level does
not changed. However, at a compressive strain of 5%, spin polarization of the Fe 3d orbital decreases, as evident from the shifts of the α and β states in PDOS (figure 7(a)), leading to a significant reduction of magnetic moment by 26.5% as compared to the unstrained Fe–MoSe₂. The magnetic moment of Co–MoSe₂ increases monotonously with increasing biaxial strain from ~5% to 5%. The reason for such a behavior is that the spin polarization of the Co 3d orbital around the Fermi level increases with increasing strain (figure 7(b)). As for Ni–MoSe₂, the magnetic moment does not noticeably change under tensile strain. In contrast, the magnetic moment of Ni–MoSe₂ initially increases to a maximum of 2.37 μₜₜ at −2% strain, and then decreases with further increasing compressive strain (figure 6). It can be concluded that the biaxial strain can effectively modulate the magnetic properties of TM–MoSe₂ by controlling spin polarization of the 3d orbitals of TM atoms.

Further, we analyzed the electronic properties of TM–MoSe₂ under biaxial strain. The electronic characteristics and band structures are displayed in figures 6 and 8. It is found that the HM can be preserved in Fe–MoSe₂ in a strain range from −4% to 5%, while an interesting transition from HM to SGS takes place at a compressive strain of −5%. The Co–MoSe₂ preserves its SGS behavior in a strain range from −1% to 5%, but becomes HM under compressive strain larger than 1%. As for Ni–MoSe₂, HM characteristics persist at tensile strain and a compressive strain of −5%, while it shows SGS behavior in the range of compressive strain from 0% to −4%. Our results suggest that TM–MoSe₂ remains the robust SGS/HM system regardless of the biaxial strain value. We checked the electronic properties of TM–MoSe₂ under strain using the PBE + U functional, as shown in table S2. It is found that TM–MoSe₂ also preserves the HM or SGS properties.

4. Conclusions

In summary, we have systematically investigated the electronic and magnetic properties of TM–MoSe₂ by means of DFT calculations. It is demonstrated that MoSe₂ sheet with Fe/Ni impurities shows the HM character, whereas Co–MoSe₂ exhibits an SGS behavior. Interestingly, the SGS/HM of TM–MoSe₂ can be well preserved regardless of biaxial strain value. In addition, Fe, Co, Ni atom substitutional impurities can induce magnetism in MoSe₂ monolayer. The magnetic moments of TM–MoSe₂ can be effectively tuned under the biaxial strain by controlling spin polarization of the 3d orbitals of Fe, Co, Ni atoms. Experimentally, strain engineering of 2D materials can be achieved by lattice constant mismatch, thermal-expansion mismatch, or transferring them on a flexible substrate and directly stretching, compressing, or bending the substrate [60]. Our results offer a new route to designing the SGS/HM properties and modulating magnetic characteristics of TM–MoSe₂ system and may also facilitate the implementation of SGS/HM behavior and realization of spintronic devices based on other 2D materials.

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