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The magnetic, optical and electronic properties of Mn–X(X = O, Se, Te, Po) co-doped MoS2 monolayers via first principle calculation

Qi-Zhi Lang1,2,3,*, Yan-Bin Huang1,2,3, Jie-Min Wei1,3,4, Yi Wang1,2,3, Xiang Guo1,2,3, Zi-Jiang Luo1,2,3 and Zhao Ding2,3,*

1 College of Big Data and Information Engineering, Guizhou University, Guiyang 550025, People’s Republic of China
2 Key Laboratory of Micro-Nano-Electronics of Guizhou Province, Guizhou, 550025, People’s Republic of China
3 Power Semiconductor Device Reliability Engineering Center of the Ministry of Education, Guizhou 550025, People’s Republic of China
4 School of Electrical and Information Engineering, Guizhou Institute of Technology, Guizhou 550025, People’s Republic of China
5 College of Information, Guizhou University of Finance and Economics, Guiyang, 550025, People’s Republic of China
* Author to whom any correspondence should be addressed.

E-mail: zding@gzu.edu.cn

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Abstract

The magnetic and optical properties studies in monolayer transition-metal dichalcogenides have attracted attention because of the manufacture spintronic, electronic and photonic devices. This paper reported the magnetism and optical properties of Mn–O, Mn–Se, Mn–Te, Mn–Po co-doped MoS2 monolayer systems via first principle calculation, results show Mn–X(X = O, Se, Te and Po) co-doped MoS2 monolayer systems appear half-metal (HM) ferromagnet, their corresponding magnetic moments are 1.06 B, 1.04 B, 1.04 B, 1.03 B, respectively. Co-doped systems have smaller band gaps due to effective charge compensation among Mn–O, Mn–Se, Mn–Te and Mn–Po atoms. According to calculation, we find Mn–O co-doped MoS2 monolayer has the lowest formation energy in four co-doping systems. Thus the Mn–O co-doped MoS2 monolayer has the best stability. The Mn–Se co-doped MoS2 monolayer has the highest static dielectric constants ε1(ω) and ε2(ω), refractive index n(ω) and k(ω). In energy range of 0 to 1.5 eV, the transmittance of intrinsic MoS2 system is higher than that of all co-doped MoS2 systems obtained by absorption coefficient α(ω).

Introduction

Spin transport electronics is always one of the popular topics in electronics research, and the spin freedom of electrons will produce novel and highly effective logic and storage devices [1]. Among the spintronics properties, Half-Metal Ferromagnetism (HMFM) is exceptional attention because of the enormous value in spin filter development [2, 3]. This property has been confirmed and applied to oxides [4], sulfides [5] and graphene nanorods [6], nevertheless, its application in two dimensional (2D) materials is rare.

Now, 2D materials have attracted great regard for its endless potential in optoelectronic devices. For example, graphene, which has exceptionally perfect spin characteristics including spin transport at normal temperature and a few microns distance of spinning movement, so it was once regarded as a 2D potential unlimited material in spin transport electronic devices [7–9]. However, zero band gap of graphene limited its application in devices. On the other hand, 2D transition metal sulfides have also aroused broad research interest. Monolayer MoS2, which belonging 2D transitional metal sulfide family, is a typical representative. It is a direct band gap semiconductor, its bandwidth is 1.8 eV, it has advantages in electronic and photonic device applications [10, 11]. Since Mo atoms have unsaturated d orbitals, doping vacancies or other elements can adjust Mo atoms magnetic moments [12–14]. Compared to graphene, the properties of MoS2 monolayers will change significantly. One of outstanding diversification is that there is no inversion symmetry in monolayer MoS2. But this change can arouse the valley Hall effect. Once applying an in-plane electric field, these carriers in different valleys migrate to another transverse edges [15], and the valley dependent optical selection rules were found in
monolayer MoS₂ [16]. Besides, the d orbitals of Mo atoms make MoS₂ having intensive spin–orbit coupling (SOC) effect, supposing this effect disappearing, MoS₂ will replace graphene to play a key role in exploration semiconductor electronics [17, 18].

Many works have been put forth to study magnetic properties in MoS₂ doped with transition metal(TM) [19–22]. Currently, central issue of this work is mainly on the induction of semiconductors in magnetism and manipulating magnetic stability of 2D materials. It has been confirmed that to produce 2D materials with stable magnetic properties by doping method [23, 24]. For example, substitutional of Mo with TM atoms may induce significant magnetic properties in MoS₂ monolayer [25–28], in case there is a certain distance between doped atoms [29], moreover, the magnetic coupling behavior and effects in doped 2D materials raise a valuable topic for fundamental physics and spintronic applications.

Kong [30] explored the O-doped MoS₂ single-layer system and found that the band gap width of the system decreases with increasing O-doping concentration and changes from direct band gap to indirect band gap after doping. Cao [31] explored the V, Cr, Mn doped MoS₂ single-layer system and found that the Mn-doped system is more stable than V and Cr, and shows stable ferromagnetism at room temperature. Li et al [32] investigated the absorption peak broadened in visible light of single-layer MoS₂ after Se doping, and red shift, the visible light absorption efficiency enhancement. Whereas, single atom doping only changes or enhances in one of the characteristics. It is difficult to consider multiple aspects of the characteristics at the same time. However, it is a feasible way to adjust doping system properties by co-doping. Xie et al [33] explored Mn-X (X = F, Cl, Br, At) co-doped WS₂ monolayer system and found that Mn-doped, Mn-Br co-doped WS₂ system changed to be completely (100%) spin-polarized HMFM, Mn-X co-doping system show better optical and gas sensing property. Nevertheless, it is seldom reported in this aspect of Mn-X (other family elements) co-doping MoS₂ monolayer system to regulate electronic structure, magnetic, and optical properties. Thus, one can expect to carry out detailed research and obtain good characteristics of semiconductor by Mn-X (X = O, Se, Te, Po) co-doping (using a X atom to replace a Mo atom and its nearest-neighbor S atom, respectively) MoS₂ monolayer both in magnetic and optical properties in order to gain deep understanding of transitional metal dichalcogenides.

Computational methods

Our calculation mainly discusses four co-doped systems, the calculation of structural optimization is fulfilled by adopting Cambridge Sequential Total Energy Package (CASTEP). Computational theory is Density Functional Theory (DFT) [34]. The exchange and correlation potential of electron–electron is treated by the generalized gradient approximation (GGA) [35–37]. Ultrasoft pseudo–potentials are used for the electron-ion interactions due to their high efficiency in structural calculation and electronic properties [38]. Setting the kinetic cutoff energy of 470 eV will ensure convergence and high-accuracy of our calculation. Geometry optimization structures are plotted in figure 1. The intrinsic monolayer MoS₂ is also calculated for comparison and results are plotted in figure 1 (a). Setting the vacuum space of 16 Å will eliminate the interaction between two neighboring monolayers, both of the cells in the axial direction and the atomic positions are fully relaxed until the tolerances for the geometry optimization of a total energy within 0.5 × 10⁻⁵ eV atom⁻¹, a maximum Hellmann–Feynman force within 0.01 eV Å⁻¹, the maximum displacement was set to 0.002 Å. And the Monkhorst–Pack 5 × 5 × 1 k-points grid sampling was adopted for Brillouin zone in geometry optimizations. We adopt 4 × 4 × 1 super cells of MoS₂ monolayer with a = b = 12.66 Å in all calculations [25, 39, 40]. The spin–orbit coupling (SOC) was considered for each calculation. When performing magnetic calculations the Magnetic properties of Mn–X (X = O, Se, Te, Po) co-doped MoS₂ monolayers, spin polarization is set in advance. For all co-doped structures, the lattice parameters were obtained after the optimization of the unit cell.

Results and discussion

Optimization structure stabilities
The formation energy plays an important role in stability of doped structure and completion in our calculation. After co-doping, we used the following equation to calculate the formation energy of co-doping structures. This equation has been proven to be applicable to the formation energy calculation of any form of semiconductor material [41–43]:

\[ E_{\text{form}} = E_{\text{total}}[X] - E_{\text{total}}[\text{MoS}_2] - \sum n_i E_i \]

\( E_{\text{total}}[\text{MoS}_2] \) represents total energy of intrinsic MoS₂ monolayer. \( E_{\text{total}}[X] \) represents total energy of X doped. \( n_i > 0 \) represents the number of atoms doped into intrinsic MoS₂ monolayer. \( n_i < 0 \) represents the number of substitution atoms of intrinsic MoS₂ system. \( E_i \) represents single atom energy. The lower formation energy of co-
doping structure, the more stable this structure. For the situation of Mn and O, Se, Te and Po co-doped MoS\(_2\) monolayers in our study, their corresponding formation energy values are 2.14, 2.63, 3.38 and 4.26 eV, respectively. These calculation results indicate that the structure of the Mn–O co-doped has the best stability.

**Electronic and magnetic properties**

The spin-polarized band structures of the Mn-X\((O, \text{Se, Te and Po})\) co-doped MoS\(_2\) monolayer system are plotted in figure 2. The intrinsic MoS\(_2\) monolayer system reveals the character of nonmagnetic semiconductor, and their band structures show a perfect symmetric structures. Because the spin-up channel is exactly the same as the spin-down channel. The band gap value of intrinsic MoS\(_2\) monolayer is 1.738 eV, and this value is consistent with \[44\]. After doping Mn and Mn-X\((X = \text{O, Se, Te and Po})\) co-doping, metallic character appeared in doped system due to the spin-up channel having some impurity bands, indicating that the Mn–O, Mn–Se, Mn–Te, Mn–Po co-doped MoS\(_2\) monolayer system become an HMFM semiconductor with a complete (100\%) spin polarization, which indicates a great potential and value in the spintronic device. Table 1 shows mainly band gaps of the intrinsic, Mn and Mn-X\((O, \text{Se, Te and Po})\) co-doped MoS\(_2\) monolayer systems.

After energy calculation, figure 3 shows the partial density of states (PDOS) diagram of all MoS\(_2\) systems of our calculation, the black line represents the total density of states (TDOS). The PDOS projecting onto doped atoms Mn-3d, Mo-4d, S-3p and X-p with intrinsic, Mn doped, Mn-X\((O, \text{Se, Te, Po})\) co-doped MoS\(_2\) monolayer are also shown in figure 3. The intrinsic MoS\(_2\) monolayer has wide conduction band, the distribution range of energy mainly between 1.50 to 15.34 eV, we can obtain that this intrinsic semiconductor system reflects nonmagnetic, because its channels have perfect symmetry with spin-up and spin-down. Figure 3(b) shows the TDOS in the Mn doped MoS\(_2\) monolayer, which has a magnetic HM character with a complete (100\%) spin polarization at the Fermi level [33]. The origin of magnetic HM is mainly that there is only a few partial-occupied impurity state in the spin-up channel. It’s PDOSs show these impurity states are mostly originated from Mn-3d state hybridized with Mo-4d state.

After doping MoS\(_2\) monolayer systems, Mn doped MoS\(_2\) appears magnetic due to the electrons in the \(d\) shell of Mn atoms were distributed spin asymmetric with the electronic configuration of Mn changing from 3d\(^5\)4s\(^2\) to 3d\(^3\). To research the magnetism of Mn-X\((O, \text{Se, Te and Po})\) atoms co-doped MoS\(_2\), using Mn-X atoms to replace Mn atoms, X\((O, \text{Se, Te and Po})\) atoms will capture 2 electrons from Mn atom for obtaining X\(^2^-\). While Mn provide 4 electrons to X\((O, \text{Se, Te and Po})\) atoms, its electronic configuration will become 3d\(^3\). The remaining 3 electrons of d shell were also distributed spin asymmetric, it leads to Mn and Mn-X\((O, \text{Se, Te and Po})\) atoms co-doped MoS\(_2\) still maintaining magnetism, and their magnetic moments are 0.94 \(\mu_B\), 1.06 \(\mu_B\), 1.04 \(\mu_B\), 1.04 \(\mu_B\), 1.03 \(\mu_B\), respectively.

According to the study of Xiao et al[9], the spin-valley coupling may make logic operations between valley index and spin index. The metal \(d\) orbitals in monolayer MoS\(_2\) produce the spin–orbit interaction. Due to
doping systems revealing valley Hall and spin Hall effects, the doped MoS$_2$ monolayer may appear the spin-valley coupling, which can protect valley index and spin index. Moreover, the electrons of d shell of Mn atoms in Mn doped and Mn-X(O, Se, Te and Po) atoms co-doped MoS$_2$ monolayer all are distributed spin asymmetric, which may lead to Mn doped and Mn-X(O, Se, Te and Po) atoms co-doped MoS$_2$ monolayer exist the spin-valley coupling, so Mn-X(O, Se, Te and Po) atoms co-doped MoS$_2$ monolayer will be used as a 2D promising material in the integrated spintronic and valleytronics applications.

Figure 2. Spin-polarized band structures with intrinsic, Mn doped, Mn-X(O, Se, Te and Po) co-doped MoS$_2$ monolayer system.

Table 1. The structure parameter of intrinsic, Mn mono-doped, Mn-X(O, Se, Te and Po) co-doped MoS$_2$ monolayer systems, band angle $\theta$, band length $d$, magnetic moment $M_{tot}$, and band gap of spin-up (spin-down) channels with all systems.

| System     | $d_{\Gamma-Mo}$ (nm) | $d_{M-K}$ (nm) | $\theta_{\Gamma-Mo-S}(^\circ)$ | $\theta_{M-K-S}(^\circ)$ | $M_{tot}(\mu_B)$ | $E_{g-SU}$ (eV) | $E_{g-SD}$ (eV) |
|------------|----------------------|----------------|-------------------------------|--------------------------|------------------|----------------|----------------|
| Intrinsic  | 2.407                | —              | 82.240                        | 0                        | 1.738            | 1.738          |                |
| Mn–O       | 2.593                | 1.974          | 75.389                        | 81.219                   | 0.96             | 0.396          | 0.396          |
| Mn         | 2.411                | —              | 81.847                        | 82.363                   | 0.94             | 0.150          | 0.150          |
| Mn–Se      | 2.412                | 2.444          | 82.225                        | 82.634                   | 0.94             | 0.092          | 0.092          |
| Mn–Te      | 2.412                | 2.661          | 83.912                        | 83.227                   | 0.94             | 0.154          | 0.154          |
| Mn–Po      | 2.410                | 2.760          | 84.263                        | 83.956                   | 1.03             | 0.147          | 0.147          |
Optical properties
Semiconductor material optical properties in the linear response range are often described with complex dielectric functions $\varepsilon_1(\omega) + i\varepsilon_2(\omega)$. The imaginary part $\varepsilon_2(\omega)$ with arising from interband transitions, we obtained it from calculating electronic structure of the study system in the long wavelength limit. The real part $\varepsilon_1(\omega)$ represents dielectric constant value. This value was obtained by Kramers-Kronig dispersion relationship satisfy the imaginary part $\varepsilon_2(\omega)$ [45–47].

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} p \int_0^\infty \frac{\varepsilon_2(s)}{s^2 - \omega^2} ds$$

Where $p$ is Integral value

$$p \int_0^\infty = \lim_{\delta \to 0} \left( \int_0^{\omega - \delta} + \int_{\omega + \delta}^\infty \right)$$

The refractive index of the absorption dielectric is also described by the complex refractive index $\varepsilon(\omega) = n(\omega) + ik(\omega)$. $n(\omega)$ represents the real part. The imaginary part $k(\omega)$, in relating to the absorption of the dielectric, called the extinction coefficient.

Figures 4(a) and (b) respectively show the calculation $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ of dielectric constant $\varepsilon(\omega)$ with intrinsic, Mn doped, Mn–O, Mn–Se, Mn–Te and Mn–Po co-doped MoS$_2$ monolayers. As shown in figure 4(a),
the static dielectric constants $\varepsilon_0(0)$ are 6.125, 8.841, 6.576, 11.083, 7.116 and 7.124 with intrinsic, Mn doped, Mn–X (O, Se, Te, Po) co–doped MoS$_2$ monolayers. These results suggest that the static dielectric constant $\varepsilon_0(\omega)$ of intrinsic MoS$_2$ monolayer is the lowest in all systems in our calculation. On the other hand, the static dielectric constant $\varepsilon_0(0)$ of Mn–Se co–doped MoS$_2$ is the highest in all doped systems, and its $\varepsilon_0(0)$ is 1.954. With observing the enlargement of the rectangle areas in figure 4(a), in the photon energy range of 0 to 2.5 eV, the $\varepsilon_1(\omega)$ of doped MoS$_2$ systems decrease firstly and then increase together with the intrinsic MoS$_2$; until the peak values of 8.613, 7.581, 7.540, 8.285, 1.917 eV and 1.876 eV of the intrinsic, Mn doped, Mn–O, Mn–Se, Mn–Te and Mn–Po co–doped MoS$_2$ monolayers. With continuously increasing photon energy, the $\varepsilon_1(\omega)$ of the calculation systems decreases again. In the energy range of 5.26–7.70 eV, $\varepsilon_1(\omega)$ become negative. When $\varepsilon_1(\omega) > 0$, photons spread from materials, while $\varepsilon_1(\omega) < 0$, the electromagnetic wave is weakened, once $\varepsilon_1(\omega) = 0$, only longitudinally polarized waves will appear. In figure 4(b), it reveals the $\varepsilon_2(\omega)$ increases with increasing photon energy, the maximum values of imaginary parts appeared near 2.91 eV, except for Mn doped and Mn–Se co–doped MoS$_2$ systems, their $\varepsilon_2(\omega)$ values decrease when the energy increase from 0.08 to 0.82 eV and 0.05 to 0.94 eV due to their HM character as mentioned above.

Figures 4(c) and (d) show the real part $n(\omega)$ and the imaginary part $k(\omega)$ of the refractive index with intrinsic, Mn doped, Mn–O, Mn–Se, Mn–Te, Mn–Po co–doped MoS$_2$ monolayers. It finds that the $n(\omega)$ and $k(\omega)$ is the same with the $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, respectively. We obtain static refractive indices $n(0)$ are 2.475, 2.979, 2.564, 3.342, 2.668 and 2.670 for intrinsic, Mn doped, Mn–X (O, Se, Te and Po) co–doped MoS$_2$ monolayers from figure 4(c). As shown in figure 4(d), by increasing photon energy in the range of 0–5.5 eV, the $k(\omega)$ is increasing up to the highest values of 1.537, 1.494, 1.494, 1.492, 1.532 and 1.533 for intrinsic, Mn doped, Mn–X (O, Se, Te and Po) co–doped MoS$_2$ monolayers. Nevertheless, there are two exceptions for Mn doped and Mn–Se co–doped MoS$_2$ systems, for HM character, which $k(\omega)$ values decrease with increasing photon energy in range of 0.16–0.82 eV and 0.16–0.94 eV due to HM character as mentioned above, and their $k(\omega)$ value increases with increasing photon energy from 0.824 eV and 0.942 eV up to the maximum value of 1.494 and 1.492, their energy
reached at 3.421 eV and 3.508 eV. At the same time, the $k(\omega)$ of the calculated systems has an oscillation behavior in the photon energy range of 3.2 eV to 6.5 eV. In figure 5, we can find that the maximum absorption peaks are 12.407, 11.783, 11.813, 11.850, 12.059 and 12.044 for the photon energies at 6.442, 6.484, 6.296, 6.422, 6.353, 7.116 and 6.347 eV with intrinsic, Mn doped, Mn-X (O, Se, Te and Po) co-doped MoS$_2$ monolayers, respectively. In the energy region of 0 to 1.5 eV, doped systems have larger absorption compared with the intrinsic MoS$_2$ monolayer systems. This result suggests the intrinsic MoS$_2$ monolayer system has the highest transmittance in the range of 0 to 1.5 eV. Besides, absorption $\alpha(\omega)$ of the intrinsic MoS$_2$ monolayer systems is larger than those of the doped systems in the range of 6.44 to 7.6 eV. From analyzing the enlargement of the rectangle areas in the energy region of 6.44 to 7.5 eV in figure 5, which shows that the performance of intrinsic MoS$_2$ monolayer systems is more excellent in the manufacture of near-ultraviolet (6.44–7.5 eV) photodetector. Meanwhile, Mn doped, Mn–O, Mn–Se, Mn–Te and Mn–Po co-doped MoS$_2$ monolayers will have better prospects in the field of infrared photodetector [48–50].

When the light wave propagates in a conductive medium, because there are free electrons in the conductive medium, the wave stimulates a conduction current in the medium during the propagation process, and part of the energy of the light wave is converted into Joule heat of the current. Therefore, the absorption coefficient of the conductive medium is given in the conductivity. For example, in semiconductors and metals, the amplitude of light waves gradually declines with the depth of penetration, that is, light absorption occurs. Since the Mn-X (O, Se, Te and Po) co-doped MoS$_2$ monolayer system exhibit metallic properties, light absorption will occur when light waves pass through these doped systems. The greater the refractive index, the more obvious the light absorption. Therefore, in different energy ranges, the absorption coefficient of the doped system changes differently [48]. Especially, when the value of the absorption coefficient $\alpha \approx 10^{-5}$ cm$^{-1}$, it is an effective value, in this condition, and the light absorption is actually centred on the very thin surface layer of the crystal.

**Conclusion**

We have studied the structure, electronic, magnetic and optical properties of Mn–O, Mn–Se, Mn–Te, Mn–Po co-doped MoS$_2$ monolayer systems calculated via spin-polarized first-principles calculations based on density functional theory. Results reveal intrinsic MoS$_2$ monolayer system is a non-magnetism semiconductor, Mn-X (X = O, Se, Te and Po) co-doped MoS$_2$ monolayer system reveals half-metal (HM) ferromagnet, their corresponding magnetic moments are 1.06 $\mu_B$, 1.04 $\mu_B$, 1.04 $\mu_B$, 1.03 $\mu_B$, respectively. However, these co-doped systems show good HM properties and their energy band gaps are 0.667, 0.578, 0.558 and 0.564 eV in the spin-up channel, respectively, because of the impurity level generated by doping atoms splitting around the Fermi level. Compared with the corresponding original structures, co-doped systems has smaller band gaps for effective charge compensation among Mn–O, Mn–Se, Mn–Te and Mn–Po atoms. According to calculation, we find Mn–O co-doped MoS$_2$ monolayer has the lowest formation energy in all co-doping systems. Thus this system has the best stability. The Mn–Se co-doped MoS$_2$ monolayer has the highest static dielectric constants $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, refractive indices $n(\omega)$ and $k(\omega)$. When the energy range of 0 to 1.5 eV, the transmittance of
intrinsic MoS₂ monolayer is much higher than that of other doping systems by calculation of absorption coefficient $\alpha(\omega)$.

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ORCID iDs

Qi-Zhi Lang https://orcid.org/0000-0002-2097-4748

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