

# The First-Principles Study On Mo-Doped Monolayer ReS<sub>2</sub>

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## Research Article

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## The First-Principles Study on Mo-doped Monolayer ReS<sub>2</sub>

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## Abstract

Based on first-principles calculations, the electronic structure and optical properties of the Mo-doped monolayer rhenium disulfide (ReS<sub>2</sub>) model are calculated, as well as the system stability, bond length, charge difference density, band structure, photoabsorption coefficient, system stability, and reflectivity are analyzed. The calculation results show that doping changes the structural stability of the system, which gradually decreases with an increasing concentration of doping. The calculation of bond structure and density of states is indicated that the band gap value of the system decrease continuously to zero with increasing doping concentration, while the average charge population of atoms at doping sites keeps increasing with the better electron-losing ability of atoms. Compared with the intrinsic monolayer ReS<sub>2</sub>, the peak of systemic reflectivity at different doping concentrations has corresponding degrees of redshift in a certain wavelength range, as demonstrated by the optical properties.

Key Words: ReS<sub>2</sub>, doping, bond gap, electronic structure, optical property

## 1 Instruction

Two-dimensional transition metal sulfides (TMDs) have been known since 1960. More than 40 kinds of TMD materials and their basic properties were conducted as early as 1969<sup>[1-3]</sup>, with the most topical materials in Group VI, MoS<sub>2</sub> and WS<sub>2</sub>, being the most prevalent<sup>[4,5]</sup>. Recently, rhenium disulfide (ReS<sub>2</sub>) semiconductor materials in Group VII have attracted widespread because of their undeniable enormous application potential. Rhenium disulfide (ReS<sub>2</sub>) consists of three atomic layers, S-Re-S, in which Re and S covalently bond together, and has unique structural,

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optoelectronic, and chemical properties that have led to subsequent studies of various properties of rhenium disulfide [6-14].

In the design and application of nano-devices, the tunability of the band gap is essential for materials. Rhenium disulfide, which exhibits semiconducting transition metal properties, cannot be effectively used in micro- and nano-devices yet. Thus, its modification has become a research hotspot. There have been many researchers to modulate the intrinsic properties of rhenium disulfide such as band gap, transport characteristics, and magnetic properties by adsorption, stretching, and straining [15-18]. Rhenium disulfide has no transition from direct to indirect band gap, making it unique among semiconductor transition metal dihalides, while atomic substitutional doping becomes a new feasible strategy due to its effective modulation for band gap. Meantime, transition metal sulfides have received increasing attention as electrochemical energy storage and electrode conversion materials for lithium-ion batteries and hydrogen evolution reactions, and so on. However, most of them show a low electrical conductivity, which significantly limits their electrochemical performance. Therefore, metal heteroatom doping can be used for modulating the electronic structure, which is an effective strategy to solve this problem.

Deniz et al.<sup>[19]</sup> studied the structural, electronic, and magnetic properties of substitutionally doped ReS<sub>2</sub> monolayers at either the S or Re site systematically via first principles density functional calculations, confirming that Mo, Nb, Ti, and V atoms can be easily incorporated in a single layer of ReS<sub>2</sub> as substitutional impurities. This particular phenomenon aroused an interest in the field, and the substitutional doping of rhenium disulfide was also conducted through experiments. Zheng and the co-workers<sup>[20]</sup> investigated the optical properties of Au-doped ReS<sub>2</sub> using piezoreflectance (PzR) measurements. They characterized the polarization property and identified the origin of the excitonic transitions as well. Obodo et al.<sup>[21]</sup> proved that a ferro- or a non-magnetic ground state constructure could be obtained by choosing dopant ions in ReS<sub>2</sub> and ReSe<sub>2</sub> monolayers with the method of quantum mechanical calculations. Liang et al.<sup>[22]</sup> prepared Au-doped ReS<sub>2</sub> layer crystals by chemical vapour method, analyzing the impact of Au in the conductivity, anisotropy,

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and photoconductivity spectra of doped ReS<sub>2</sub>. After the substitutional doping of rhenium disulfide by metallic elements was achieved, transition elements also aroused interests, among which molybdenum was hot. Yen et al.<sup>[23]</sup> grew Mo-doped disulfide single crystals employing chemical vapor transport method, finding that the activation energy of the impurity carriers increased with doping. Qin et al.<sup>[24]</sup> realized substitutional Mo-doped monolayer rhenium disulfide via chemical vapor deposition, promoting the application in the optoelectronics field. Wang et al.<sup>[25]</sup> optimized Mo-doped rhenium disulfide nanosheets anchored on brush-like carbon arrays, which exhibited excellent electrochemical properties. Following atomic substitutional Mo-doped rhenium disulfide, an increasing number of researchers studied its photoelectric properties and magnetism. However, few studies have focused on the effect of different doping concentrations on the band gap evolution and electronic structure of rhenium disulfide supercell. Do rhenium disulfides optimized by substitutional Mo-doping exhibit new properties at different doping concentrations, and does the band gap change regularly? Al-Dulaimi et al.<sup>[26]</sup> synthesized polycrystalline thin films of Mo-doped rhenium disulfide alloys via aerosol-assisted chemical vapor deposition (AACVD) and found that the interlayer spacing increased and the vibrational modes of ReS<sub>2</sub> destructed with increasing Mo content in the ReS<sub>2</sub> substrate. Qin et al.<sup>[27]</sup> constructed a supercell model of ReS<sub>2</sub> to study the band gap variation at two different doping concentrations using first-principles software. Nevertheless, the above studies are merely limited to the structure, strain, and bandgap changes at different concentrations, and the effect of different concentrations of Mo atomic doping on the electronic structure and optical properties of rhenium disulfide remains to be investigated, among which whether the band structure can achieve zero band gap remains to be explored.

Herein, we systematically calculated the system, electronic structure, and optical properties of substitutional Mo-doped monolayer rhenium disulfide, which compared with pure rhenium disulfide system. Furthermore, the evolution in band gap, electronic structure, and optical properties of doped ReS<sub>2</sub> system was discussed. It is expected that our studies will provide some references in the application of

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semiconductor devices.

## 2 Computational methods and models

The calculation module used in this work was Cambridge sequential total energy package (CASTEP) in Material Studio 8.0, which optimizes and simulates monolayer rhenium disulfide under different conditions based on first-principles<sup>[28]</sup>. For the exchange-correlation energy, the Perdew-Burke-Ernzerhof (PBE) functional within generalized-gradient approximation (GGA) was utilized<sup>[29-32]</sup>.

In reciprocal lattice, the first Brillouin Zone (K-points) was divided into  $7 \times 7 \times 1$  Monkhorst-Pack grid for batch calculation with the plane wave cutoff energy of 400 eV to ensure favorable convergence during the calculation. The following thresholds were used for convergence of the structure: energy iteration convergence accuracy of  $1.0 \times 10^{-6}$  eV/atom for individual atoms; internal stress convergence value of 0.05 GPa; interatomic interaction forces less than 0.01 eV/Å; and displacement of atoms less than 0.001 Å during geometry optimization.

The following thresholds were used for the convergence of structure: energy iteration convergence accuracy of  $1.0 \times 10^{-6}$  eV/atom for individual atom; internal stress convergence of 0.05 GPa; the interaction force convergence between atoms less than 0.01 eV/Å; and displacement of atoms less than 0.001 Å during geometry optimization.

A (4×4×1) supercell model of rhenium disulfide constructed using MS is shown in Fig. 1a, for a single cell of rhenium disulfide with total 3 atoms. Fig. 1b-d show the supercell models with the number of Mo atoms substitutionally doped at one, two, and three, respectively.

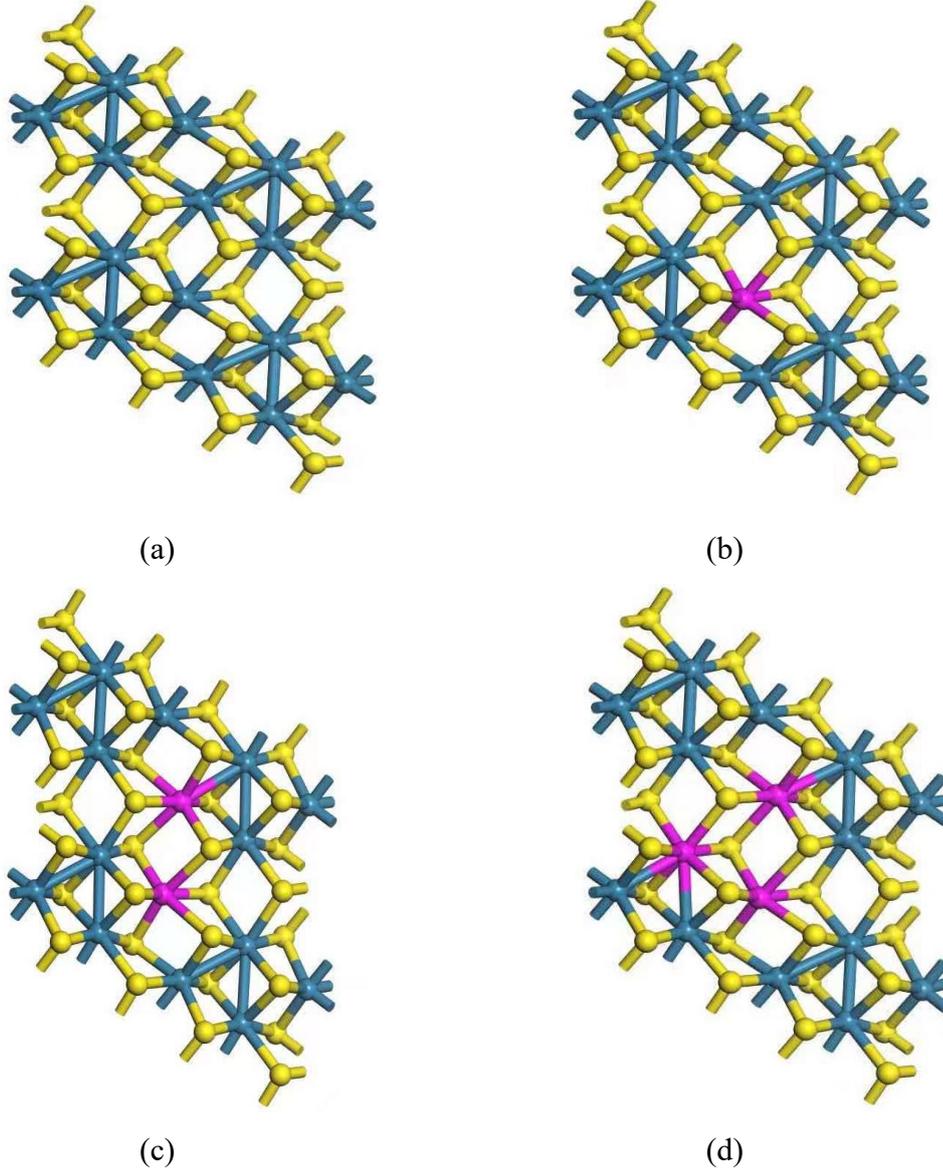


Fig. 1 ReS<sub>2</sub> model of doped without Mo atom (a) and with one Mo atom (b), two Mo atoms (c), and three Mo atoms (d).

### 3 Calculated results and models

#### 3.1 Stability of doping system

We calculated the formation energy and binding energy of doped ReS<sub>2</sub> system in order to investigate the structural stability. The formation energy is defined as shown in Eqs. (1) <sup>[33]</sup>:

$$E_{\text{form}} = E_{\text{tot}}[\text{X}] - E_{\text{tot}}[\text{ReS}_2] - \sum niE_i \quad (1)$$

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Where  $E_{\text{tot}}[\text{X}]$  and  $E_{\text{tot}}[\text{ReS}_2]$  are the total energy after doping and without doping, respectively. When  $n_i > 0$ , defined as the number of atoms doped into the system, while  $n_i < 0$  means the number of atoms removed from the system.  $E_{\text{form}}$  is the system formation energy, where a negative value indicates a stable structure, and a positive value indicates that the structure exists but requires energy to maintain it. The formation energy is calculated as 1.4116 eV, 2.3871 eV, and 3.8252 eV for Mo atom doping concentrations of 1, 2, and 3, respectively, indicating that the structure after Mo atom substitution doping still needs the energy to maintain and increases with the doping concentration. Compared with the intrinsic monolayer rhenium disulfide, the more atoms doped, there is greater the effect on the formation energy.

### 3.2 Crystalline structure

The bond length of the rhenium disulfide system will be inevitably affected by doping with Mo atoms. And its distribution of rhenium disulfide structure was discussed by numbering the atoms of the rhenium disulfide model as shown in Fig.2. It is found that the bond length with the surrounding atoms were distorted owing to doping with Mo atoms and changed at different sites.

The bond length of the Mo atoms substitutional doped at different concentrations with the surrounding S atoms with farthest distance are 2.55646 Å, 2.58808 Å, and 2.60870 Å, with the relative changes of 2.06%, 3.32%, and 4.14%, respectively, corresponding to one, two, three Mo atoms doped, respectively, as observed in Table 1 which presents the structure parameters of pure ReS<sub>2</sub> and system optimized by substitutional Mo-doped at different concentrations. It is demonstrated that the bond length and the corresponding amount of change gradually increase as more number of doped atoms, as a result of the more intense energy transfer, and the bond length change may be also relative to the band gap change to some extent.

Table 1 Bond length of Mo1-S15 in doped monolayer ReS<sub>2</sub> system

<i>System</i>	$d_{\text{Mo-s}}/\text{\AA}$	<i>Variation</i>
Re <sub>16</sub> S <sub>32</sub>	2.5049	0
Re <sub>15</sub> S <sub>32</sub> Mo	2.55646	2.06%
Re <sub>14</sub> S <sub>32</sub> Mo <sub>2</sub>	2.58808	3.32%
Re <sub>13</sub> S <sub>32</sub> Mo <sub>3</sub>	2.60870	4.14%

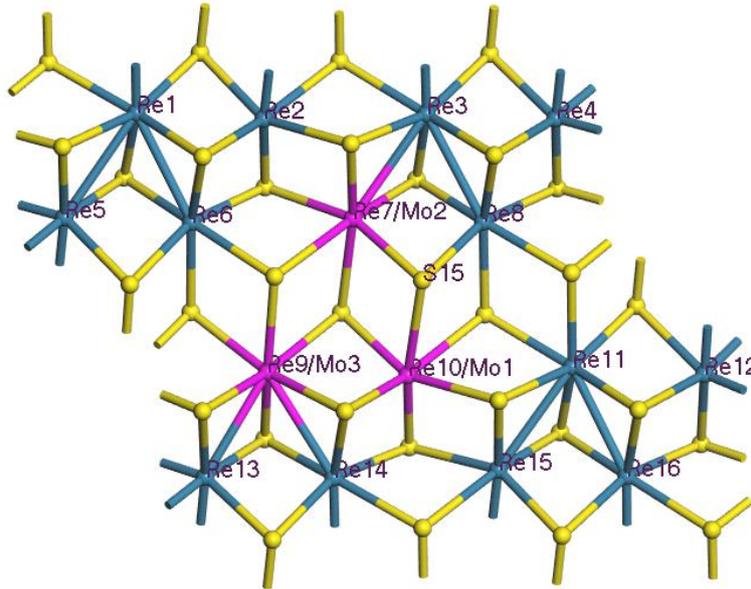


Fig. 2 Atom number

### 3.3 Influence of substitutional Mo-doping on rhenium disulfide

The electronic property of the intrinsic rhenium disulfide and Mo-doped rhenium disulfide systems were calculated using CASTEP, and the first Brillouin zone used was the closed path  $G(0,0,0) \rightarrow M(0,0.500,0) \rightarrow K(0.333,0.333,0) \rightarrow G(0,0,0)$ . Figure 3 shows the energy band structure and for intrinsic monolayer rhenium disulfide, where the rightmost shows **density of states** regarded as the projection of the energy band structure. As shown in the figure, the intrinsic monolayer rhenium disulfide is a direct band gap semiconductor with a band gap value of 1.489 eV, which is closer to the 1.440 eV in the literature<sup>[34]</sup> with the error of only 3.4%. It is seen that

the peak **density of states** of intrinsic monolayer rhenium disulfide located at -4 eV, and the DOS curve exhibited a trough trend at the Fermi energy level with a value of zero which corresponds to the band gap of the band structure. The **density of states** structure of rhenium disulfide is also demonstrated that several energy levels in the curve other than the Fermi level also close to zero, which proves that the energy band structure of rhenium disulfide possesses a large modification space and is more suitable for application in energy band engineering.

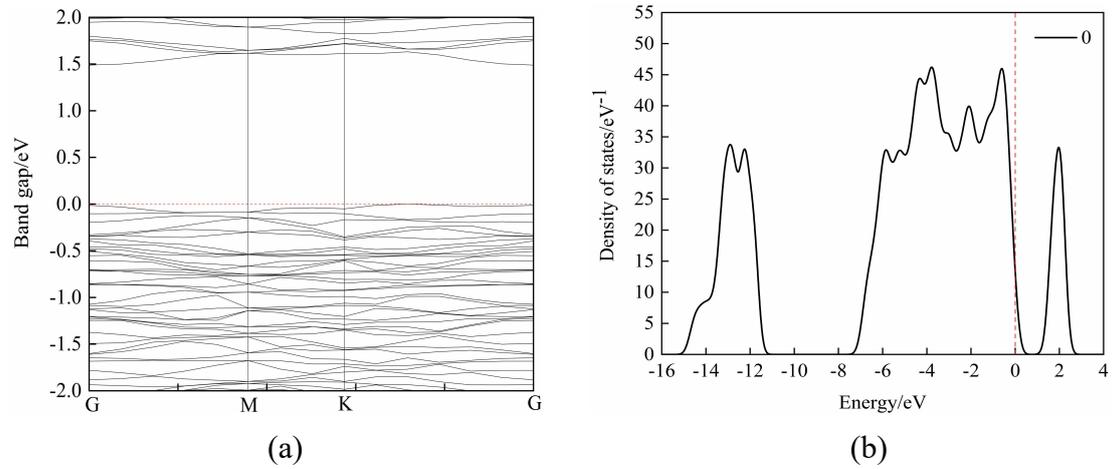
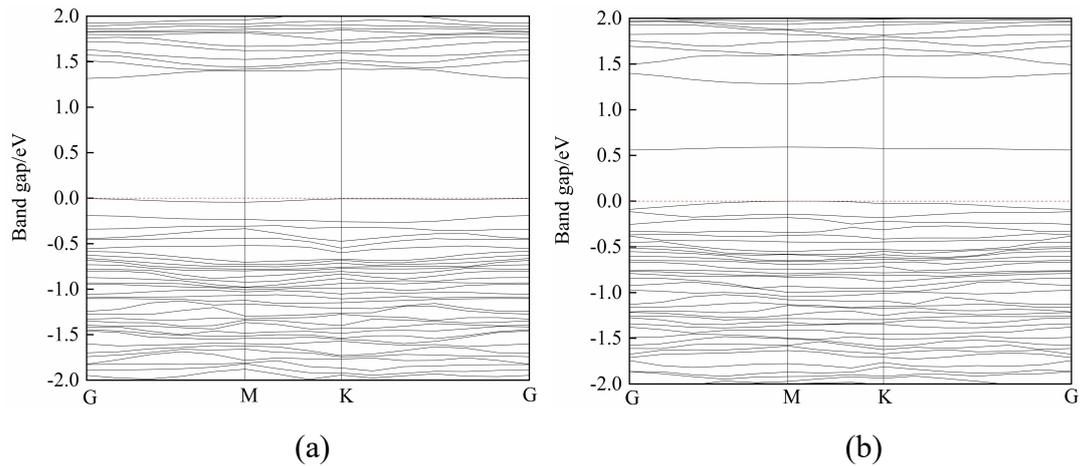


Fig. 3 Band structure (a), and structure of DOS of intrinsic rhenium disulfide (b).



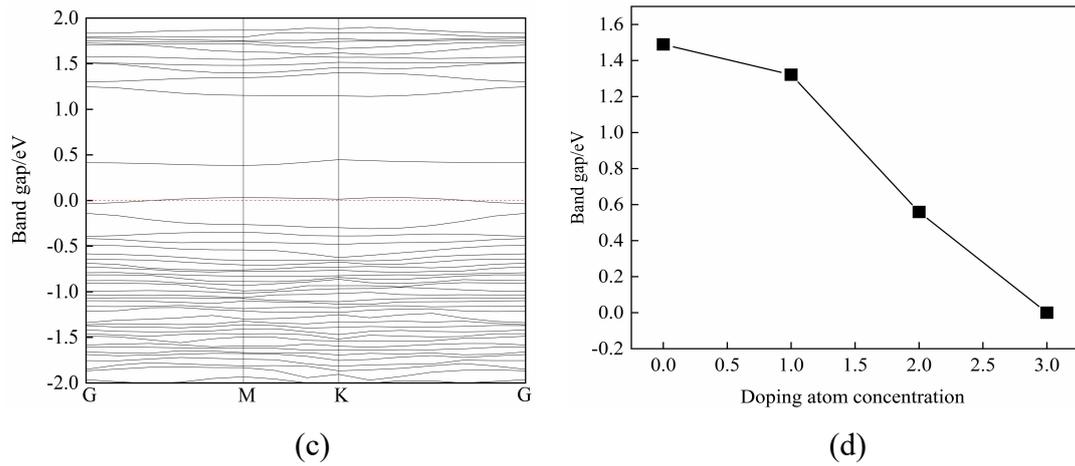


Fig. 4 Band structure of rhenium disulfide doped with one Mo atom (a), two Mo atoms (b), three Mo atoms (c), and band gap variation (d).

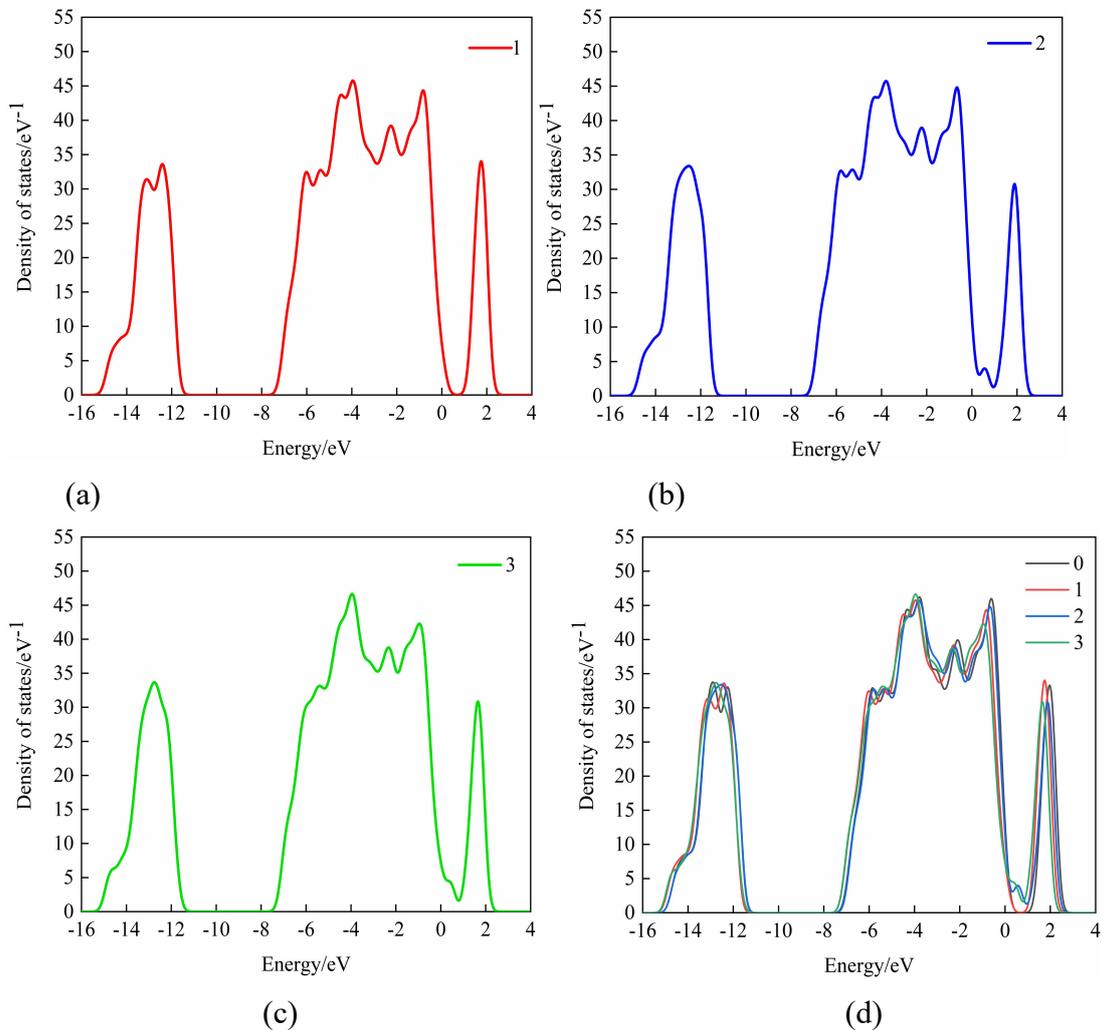


Fig. 5 DOS of rhenium disulfide doped with one Mo atom (a), two Mo atoms (b), three Mo atoms (c), and DOS variation (d).

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As can be seen from Figure 4, the band gap decreases from 1.489 eV to 1.321 eV when one Mo atom doped and continues to 0.559 eV when the number of atoms increases to two, which corresponds to a medium band gap semiconductor. When the doped atoms rise to three, the band gap decreases continuously, even eventually reaching 0 eV, corresponding to a zero gap semiconductor which makes it a material with metallicity. In the range of our current study, the band gap reduces with an increasing number of single Mo atoms doped, meaning that the minimum energy required for valence electron to guide band declines. When doped two or three atoms, the band gap value goes down more significantly with a more obviously decline of band gap, the minimum energy required for valence electron to guide band falls down more deeply. The density of states plotted for different number of doped atoms shows that the density of states of the system varies slightly with the number of doped atoms, and its range where the number of electronic states near the Fermi plane is zero shrinks with an increasing number of doped atoms, corresponding to the energy band structure.

In order to study the charge distribution and electron transfer, the charge density difference and Mulliken charge population of substitutional Mo-doped ReS<sub>2</sub> system were calculated in this paper. The charge density difference of substitutional Mo-doped ReS<sub>2</sub> system is shown in Fig. 6, and the charge population of Mo atoms and surrounding Re atoms under the effect of substitutional Mo-doping are listed in Table 2. When doped with one Mo atom, Mo1 replaces Re10; When doped with two Mo atoms, Mo1 replaces Re10 and Mo2 replaces Re7; When doped with three Mo atoms, Mo1 replaces Re10, Mo2 replaces Re7 and Mo3 replaces Re9, relatively.

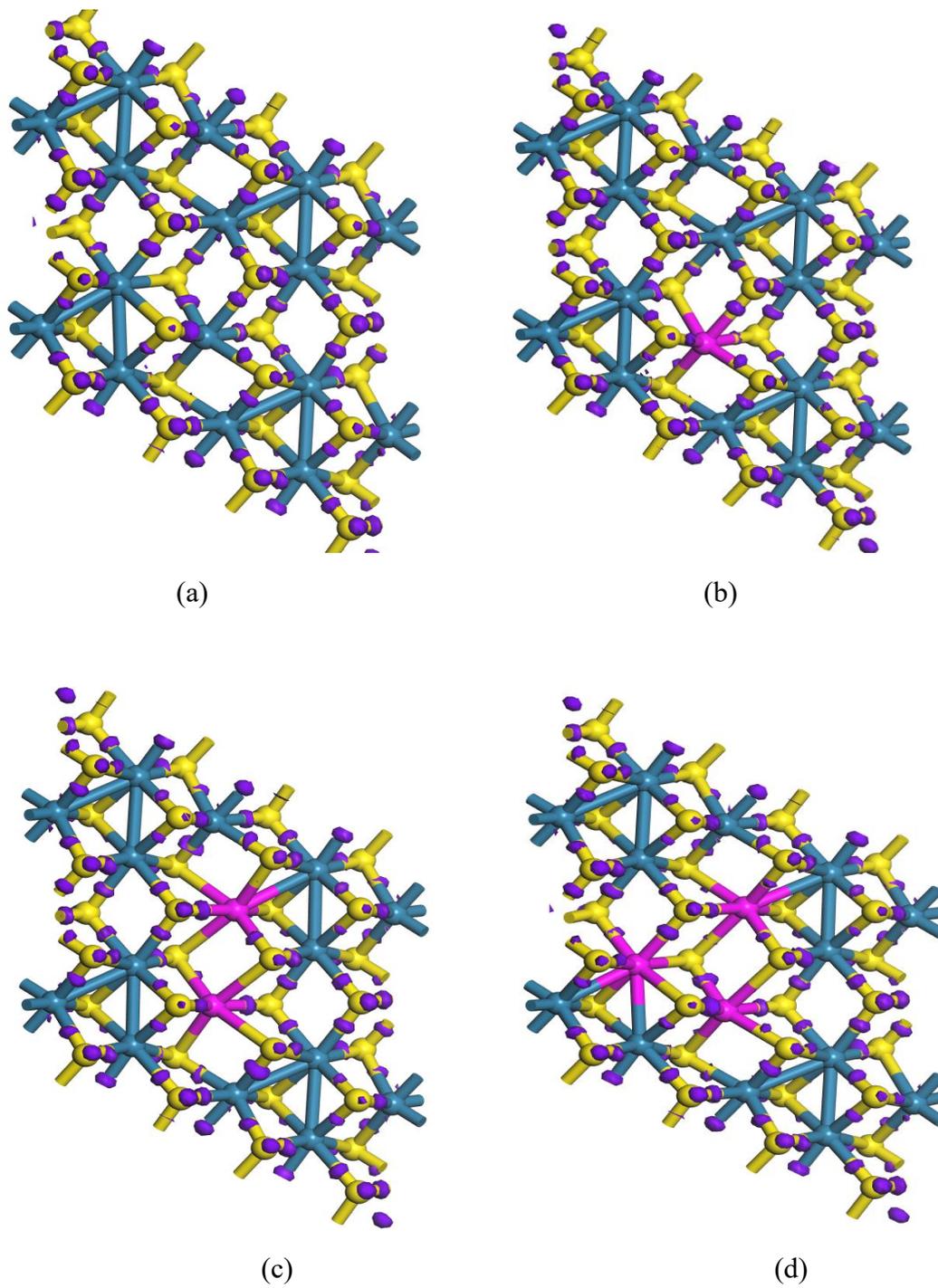


Fig. 6 The charge density difference when doped without Mo atom (a) and with one Mo atom (b), two Mo atoms (c), and three Mo atoms (d).

Table 2 The charge population of Mo atoms under the effect of substitutional Mo-doping

Mulliken Charge population				
Doped Atoms	0	1	2	3
Re3	0.23	0.23	0.17	0.19
Re6	0.23	0.23	0.21	0.17
Re13	0.16	0.16	0.16	0.19
Re14	0.23	0.20	0.17	0.15
Re7/Mo2	0.16	0.15	0.32	0.34
Re9/Mo3	0.22	0.19	0.23	0.37
Re10/Mo1	0.16	0.38	0.32	0.33
Average charge population of	0.18	0.24	0.29	0.35

Fig. 6 shows the systematic charge density difference with a different number of doped atoms, where the purple part indicates the distribution. It is seen that the distribution of charge density difference in the system with a different number of doped atoms is relatively uniform, in which the charge mainly concentrated on the bonds between Re-S and Mo-S. It can be inferred that charge transfer occurred between Re and S as well as Mo and S, which is especially manifest between the doped Mo atoms and their nearby S atoms. When the monolayer of intrinsic rhenium disulfide is doped with Mo atoms in place, the value of charge accumulation in the bonding region between the doped Mo atoms and S atoms disperses, and the electronegativity strengthens with an increasing number of doped atoms. In contrast, the charge accumulates more dramatically in the area between Re atoms and S atoms near the Mo atoms, with a mainly weakened electronegativity. Associated with Mulliken charge population, it can be observed that the charge population of doped

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Mo atoms increases to a varying degree compared to that of original Re sites in the intrinsic rhenium disulfide system. In other words, when doped with one atom, the charge population of Mo1 (formerly Re10) goes up from 0.16 to 0.38, even more than two times, with an atomic loss of 0.22 e. When doped with two atoms, the charge population of Mo1 increases from 0.16 to 0.32, and that of Mo2 (formerly Re7) also increases from 0.16 to 0.32 in comparison with the intrinsic ReS<sub>2</sub> system. Furthermore, when dopant atoms increase to three, Mo1, Mo2, and Mo3 (formerly Re9) increase to 0.33, 0.34, and 0.37, respectively, in keeping with the conclusion obtained by the charge density difference. At the same time, the average charge population of the atoms at the three doping positions has been increasing with the increase of Mo atoms doped, of which values are closer to each other. In addition, the charge between Mo and S atoms also transfers more frequently with the increase of the number of doped atoms. Simultaneously, the electron losing ability of the atoms at the three doping positions becomes stronger.

#### 3.4 Influence of substitutional Mo-doping on optical property of rhenium disulfide

To study the effect of different concentrations of Mo-doping on the optical property of the monolayer rhenium disulfide system, the curves of systematic absorption coefficient and reflectivity were plotted, as shown in Fig. 7 and 8. Meanwhile, the location (wavelength) of the highest reflection peak and absorption peak, as well as their characteristic values in the Mo-doped monolayer rhenium disulfide system, were listed in Table 3 and Table 4. It can be seen that the light starts to reflect in all doped systems at a wavelength of 63 nm from Fig. 7 a and b. the original system shows a reflection peak at a wavelength of about 188.64 nm with the value of 0.354 cm<sup>-1</sup> from Fig. 7a-b and Table 3. The increase in the number of doped atoms causes redshift of the highest reflection peak to different degrees with respect to the original ReS<sub>2</sub> system. Moreover, the light is not absorbed in the Mo-doped ReS<sub>2</sub> system with the wavelength range from 0 to 64 nm, while it starts to be absorbed when the wavelength reaches 64 nm, as illustrated in Fig. 8a and b. It is observed that the absorption coefficient of the original system grows to a maximum value of 77176.4 cm<sup>-1</sup> at a wavelength of about 369.20 nm from Fig. 8a-b and Table 4.

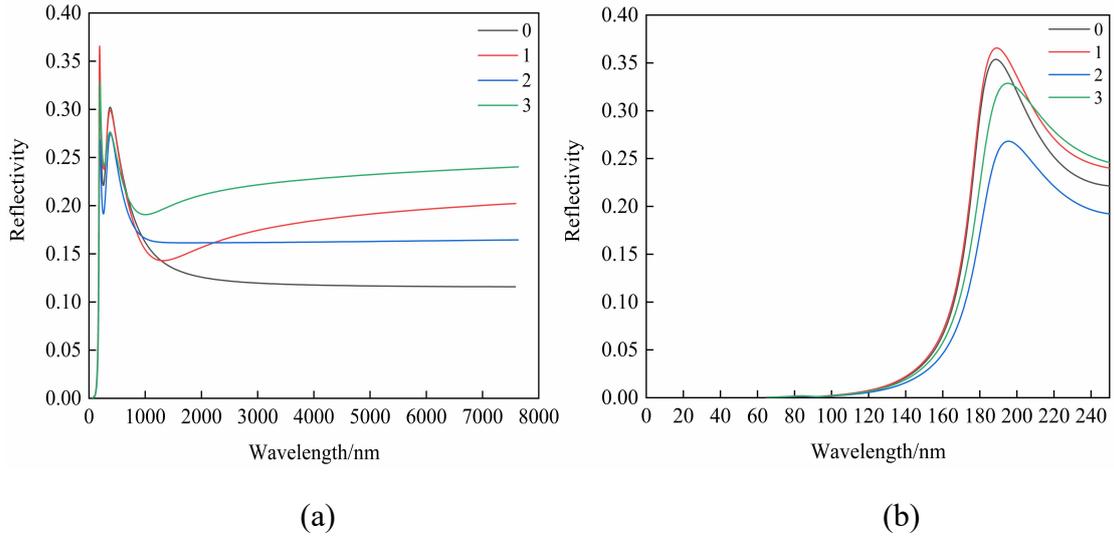


Fig. 7 Reflectivity of light under monolayer rhenium disulfide at different doping concentrations (a) and the partial enlarged detail (b).

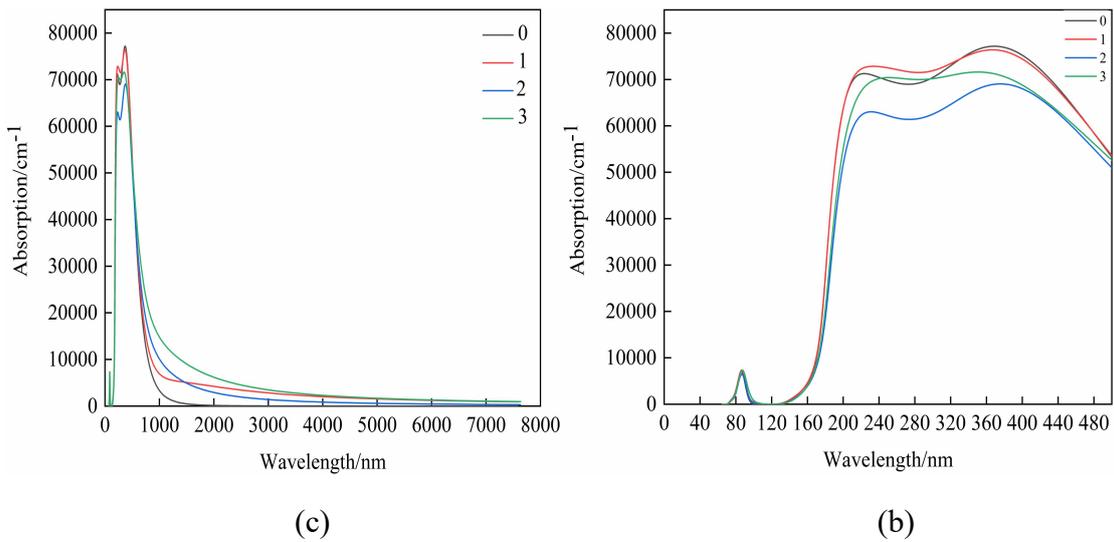


Fig. 8 Photoabsorption coefficient under monolayer rhenium disulfide at different doping concentrations (a) and the partial enlarged detail (b).

Table 3 The wavelength and characteristic value of the highest reflection peak for monolayer rhenium disulfide under substitutional Mo-doping.

Doping atoms	Wavelength /nm	Characteristic value /cm <sup>-1</sup>
0	188.64	0.353696
1	189.12	0.365639
2	195.10	0.268123
3	195.19	0.328682

Table 4 The wavelength and characteristic value of the highest absorption peak for monolayer rhenium disulfide under substitutional Mo-doping.

Doping atoms	Wavelength /nm	Characteristic value /cm <sup>-1</sup>
0	369.20	77176.4
1	366.40	76401.1
2	376.02	69054.9
3	350.89	71613.2

## 4 Conclusions

In summary, the system of ReS<sub>2</sub> doped with Mo atoms are calculated by means of density functional theory and its formation energy, and bond length are analyzed relatively to investigate the effect of Mo-doping on the stability of Res<sub>2</sub>. The results indicate an increase of formation energy and a decrease of bonding energy for ReS<sub>2</sub> when more Mo atoms doped. Namely, the stability shows a negative correlation with the number of doped atoms. The influence of doping on electronic structure is concluded by studying the bond structure, density of states, charge density difference, and charge population. Band structure and density of states studies show that the direct band gap of ReS<sub>2</sub> is not changed and the Fermi energy level cannot be moved under the effect of Mo-doping, while the band gap can be tuned. The band gap shrinks with an increasing number of Mo atoms doped, even becomes zero band gap when

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doped with three atoms, which makes it exhibit metallic properties. The charge

The analysis of charge density difference and charge population demonstrates that the charge transfer occurs on the bonds Re-S and Mo-S. The charge accumulation in the bonding region between the doped Mo atoms and S atoms disperses, and the electronegativity strengthens with an increasing number of doped atoms. The charge population of doped Mo atoms increases to a varying degree compared to that of original Re sites in the intrinsic rhenium disulfide system and the average charge population of the atoms at the three doping positions has been increasing with the increase of Mo atoms doped. It can be seen by studying the optical property that the increase in the number of doped atoms causes redshift of the highest reflection peak to different degrees with respect to the original ReS<sub>2</sub> system. The results above show that substitutional Mo-doping is less sensitive to the systematic optical property but more to the band gap value and the degree of charge transfer.

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