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NO gas adsorption properties of MoS$_2$ from monolayer to trilayer: a first-principles study

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Abstract
The NO gas adsorption properties of the monolayer, bilayer and trilayer MoS$_2$ has been studied based on the first-principles calculation. The interaction between NO and MoS$_2$ layers is weak physical adsorption, which is evidenced by the large distance (>3 Å), small adsorption energies (<0.9 eV) and deformation electron density. Moreover, the effect of the NO adsorption on the charge transfer and the electronic properties are also discussed. For all the NO adsorption cases, 0.04 e charge transfer exists by Mulliken/Hirshfeld analysis and and the charge density difference between NO molecular and MoS$_2$ layers. The NO adsorption can obviously induces new impurity states at about 0.5 eV in the band gap that can lead to the change of the transport properties of the MoS$_2$ layers and then it could detect the NO gas. We also performed semi-quantitatively theoretical analysis from the carrier concentration $n$ and carrier mobility $\mu$ to obtain the effect of the NO adsorption on electrical conductivity. Our results provide a theoretical basis for the application of MoS$_2$ layers as gas sensors for important NO polluting gases in air.

Introduction

In recent years, transition metal dichalcogenides (TMDs) have attracted much interest due to their unique layer structure and excellent electronic, optical and properties. They have been found an increasingly wide utilization in almost all fields, like sensors [1–7], field-effect transistors [8, 9], supercapacitors [10–13], photovoltaic and photocatalytic devices [14, 15], et al. Especially, MoS$_2$, as the frontrunner in TMDs material, shows high thermal stability, tunable band gap, large surface-to-volume ratio, and various active sites, which makes it a promising candidate for high-performance gas detection[2, 5, 16]. There are numerous researches focus on chemical element defect methods to improve and enhance the application as a gas sensor [5, 17, 18]. For instance, Xiaoxing Zhang et al predicted that Ni–MoS$_2$ has the potential to be used as a gas sensor for COF$_2$ detection based on the density-functional theory (DFT) calculations [19]. Dongwei Ma et al. The interaction between CO or NO with the doped MoS$_2$ monolayer is strong and belongs to the chemisorption [17]. Kala et al studied the intrinsic influence of gas sensing nature of V$_5$ and V$_{Mo}$ monolayer MoS$_2$, and found that monolayer MoS$_2$ with vacancy defect are producing beneficial results for sensing PH$_3$, BBr$_3$ and SF$_4$ gas molecules than Cl$_2$ and AsH$_3$ [20].

NO is one of the most common toxic gas molecules and is extremely harmful to human being. NO is usually releases from industries, and automobile vehicles, and it could cause acid rains when the amount of NO in the environment is high. So it is significant to detect the NO gas for a good living and working environment. Some researches show that MoS$_2$ becomes auspicious for NO gas sensor applications [17, 21, 22]. Early in 2014, Jianming Xue et al predicted that the MoS$_2$ single layer should be more sensitive than graphene when used as NO...
Recently, S Ramu et al demonstrated the NO gas sensing properties of MoS$_2$ monolayer at low temperature (27°C to 100°C) under UV light [23].

In the previous researches, especially in theoretical calculation, researchers mainly focus on only pursuing the strong adsorption (chemical adsorption) and larger charge transfer, which is beneficial for gas sensing response of sensor. However, the physical adsorption behavior of gas molecules can overcome the shortcoming of difficult desorption in two-dimensional materials, because weak adsorption could improve the recovery characteristics of gas sensors. For example, Yong Zhang et al suggested that few-layer MoS$_2$ nanosheets prepared via mechanical exfoliation exhibit high responsivity for room-temperature NO$_2$ detection, and NO$_2$ is easily desorbed from the sensor surface with an ultrafast recovery behavior, with recovery times around 2 s [2]. Moreover, some studies have shown that few-layer MoS$_2$ exhibits much higher electronic mobility compared with monolayer MoS$_2$, thus making it more suitable for gas sensor [24]. Although, Hua Zhang et al have demonstrated a highly sensitive field-effect transistor (FET) sensor based on MoS$_2$ films, and studied the number of MoS$_2$ layers on the sensor performances [25]. However, the detailed interaction between NO gas-sensing properties and layer thickness of MoS$_2$ is not clearly in their report and is worth exploring. In this work, based on the first-principles calculation, we systematically investigated the effect of NO adsorption on the geometrical, charge transfer and electronic properties of monolayer, bilayer and trilayer MoS$_2$.

### Computational methods

All the DFT calculations were performed as implemented in DMol$^3$ package of Materials Studio [26]. The exchange-correlation potential is treated with the Perdew-Burke-Ernzerh (PBE) of generalized-gradient approximation (GGA) functional [27] implemented with long-range dispersion correction via Tkatchenko and Scheffler’s (TS) method [28], which has been used in numerous 2D TMDs layers DFT calculations [19, 29–32]. The double numerical plus polarization (DNP) was used as the basis set. For geometry optimization, all the atoms are fully relaxed until the forces and the displacement are less than 0.002 Ha/Å and 0.005 Å, respectively, and the convergence threshold of total energy is 1 × 10$^{-5}$ Ha. The Brillouin zone is sampled with a grid of 5 × 5 × 1 k-points by the Monkhorst-Pack scheme method. Whereas, for the electronic properties calculations, a 13 × 13 × 1 k-point mesh is adopted. Spin–orbit-dependent interlayer interactions in TMDs have not been reported before [33, 34], thus spin–orbit couplings were not taken into account and we have tested that the inclusion of these interactions does not alter any of our conclusions.

The calculated lattice constant of MoS$_2$ monolayer is 3.184 Å, which is consistent with the other theoretical or experimental values [18]. By an optimal balance between the accuracy and cost, in our calculation, we employed a 2 × 2 × 1 MoS$_2$ supercell with a 20 Å vacuum for avoiding the interaction between different cells. Our calculated band gap of monolayer MoS$_2$ is 1.770 eV, which is within a specified tolerance range compared with other theoretical results [19] and experimental data [35].

The adsorption energy of NO gas molecule on MoS$_2$ layers is determined as

$$E_{ad} = E_{NO/MoS_2} - E_{MoS_2} - E_{NO},$$

where $E_{NO/MoS_2}$ is the total energy of NO absorbed on MoS$_2$, $E_{MoS_2}$ and $E_{NO}$ represent the isolated MoS$_2$ layers and NO molecular, respectively. Thus, negative adsorption energy represents an exothermic process. Moreover, in order to intuitively understand the adsorption character, the deformation electron density, which defined as the total density with the density of the isolated atoms subtracted, is calculated. We also analyzed the charge transfer between MoS$_2$ and NO molecular by Mulliken/Hirshfeld method and electron density difference to elucidate the interaction mechanism between NO and MoS$_2$. The electron density difference is obtained by subtracting the electron density of the isolated NO and isolated MoS$_2$ component from the electron density of the NO-adsorbed system with retaining the same atomic positions. It can be expressed by the formula

$$\Delta \rho = \rho_{NO/MoS_2} - \rho_{MoS_2} - \rho_{NO}. $$

Moreover, the band structures and partial density of states (PDOS) were calculated to explore the effect of the NO gas adsorption.

### Results and discussion

#### Structural properties of NO and MoS$_2$ layers

The structures of NO gas molecular, monolayer, bilayer and trilayer MoS$_2$ are shown in figure 1. The calculated bond length of N–O is 1.16 Å, which is close to previous published report [17, 18]. Mulliken (Hirshfeld) charge of N and O atoms is 0.038 (0.015) and −0.038 (−0.015) $e$, indicating the charge transfer from N atom to O atom in NO molecular. MoS$_2$ is a sandwich layered material in which S–Mo–S atoms are arranged in honeycomb...
structure in top view as shown in figure 1. The layers are combined by van der Waals forces, which can also be observed in figure 1 that the interlayer distance is about 2.9 Å. Because the stacking configuration of bilayer and trilayer MoS$_2$ is that the Mo atoms (S atoms) in each layer correspond to the S atoms (Mo atoms) in adjacent layer, the top views of monolayer, bilayer and trilayer MoS$_2$ are the same. This stacking configuration has been proven to be the most energy favorable [36–39].

**Structural properties of NO adsorbed on MoS$_2$**

In order to systematically study the NO gas adsorbed on MoS$_2$, five typical positions (as shown in figure 2) labeled as H (hollow site, NO is above the center of the hexagonal ring of MoS$_2$), T$_{Mo-N}$ (top site, N atom in NO is at the top of Mo atom), T$_{S-N}$ (N atom in NO is at the top of S atom), T$_{Mo-O}$ (O atom in NO is at the top of Mo atom) and T$_{S-O}$ (O atom in NO is at the top of S atom) were calculated. Tables 1–3 show the adsorption energy ($E_{ad}$ in eV), bond length of NO molecules after adsorption (d$_{N-O}$ in Å), the smallest distance between NO molecular and atoms of MoS$_2$ (h$_{NO}$ in Å) in five adsorption configurations for NO gas adsorbed on monolayer, bilayer and trilayer MoS$_2$, respectively.
For NO gas adsorbed on monolayer MoS$_2$, the bond length of the adsorbed NO is almost unchanged, indicating the weak adsorption character. The smallest distances between NO molecular and atoms of MoS$_2$ are $>3$ Å much longer than the sum of the atomic covalent radii between NO gas and MoS$_2$ layer (the atomic covalent radii is 0.92 and 0.74 Å for the N and O atoms, 1.03 and 1.36 Å for the S and Mo atoms, respectively), that further supports the weak interaction between NO gas and MoS$_2$ substrates. For the case NO gas adsorbed on bilayer MoS$_2$, we observed the similar findings. However, a relative larger bond length of TMo-N, TS-N and TS-O configurations in trilayer MoS$_2$ suggests that the N–O bond of the NO molecule is weakened by the adsorption process. Also, the distances between the NO and MoS$_2$ layer are smaller a lot. According to the definition of adsorption energy, the more negative the adsorption energy, the more energy favorable the NO adsorption system is. The highest adsorption energies for monolayer, bilayer and trilayer MoS$_2$ are $-191.1$ meV (for TS-N configuration), $-214.7$ meV (for TMo-O configuration) and $-76.6$ meV (for H configuration), respectively, indicating the most favorable position for NO gas adsorbed on different thickness of MoS$_2$ layers. In the following, we mainly focus on these three configurations. Besides, our calculated NO adsorption energies of monolayer MoS$_2$ match with the other reported values well [21, 40, 41], and all the calculated adsorption energies are less than 0.9 eV, further confirming the physisorption characteristic.

**Electronic properties of NO adsorbed on MoS$_2$**

Figures 3–5 present the most stable adsorption configurations of NO gas on monolayer, bilayer and trilayer MoS$_2$ after geometry optimization. In this section, we will discuss in detail the charge transfer and electronic properties of the adsorption of NO gas on different thickness of MoS$_2$. For the NO molecular on the surface of monolayer MoS$_2$, after optimization, the NO molecular moved to the top of the Mo–S bond and the N–O bond has an angle of $38.85^\circ$ with MoS$_2$ layer, as shown in figure 3(a). The deformation electron density in figure 3(b) make more explicit description of the physisorption characteristic that there are no net charge distribution.

| Adsorption positions | $E_{ad}$ (meV) | $d_{N-O}$ (Å) | $h_{NO}$ (Å) |
|----------------------|----------------|---------------|---------------|
| H                    | $-157.9$       | $1.15$        | $3.137$       |
| TMo-N                | $-158.6$       | $1.16$        | $3.059$       |
| TS-N                 | $-191.1$       | $1.16$        | $3.145$       |
| TMo-O                | $-159.2$       | $1.15$        | $3.231$       |
| TS-O                 | $-190.7$       | $1.15$        | $3.406$       |

| Adsorption positions | $E_{ad}$ (meV) | $d_{N-O}$ (Å) | $h_{NO}$ (Å) |
|----------------------|----------------|---------------|---------------|
| H                    | $-213.8$       | $1.16$        | $3.300$       |
| TMo-N                | $-213.2$       | $1.16$        | $3.070$       |
| TS-N                 | $-86.1$        | $1.16$        | $3.060$       |
| TMo-O                | $-214.7$       | $1.16$        | $3.266$       |
| TS-O                 | $-213.7$       | $1.16$        | $3.350$       |

| Adsorption positions | $E_{ad}$ (meV) | $d_{N-O}$ (Å) | $h_{NO}$ (Å) |
|----------------------|----------------|---------------|---------------|
| H                    | $-76.6$        | $1.16$        | $3.170$       |
| TMo-N                | $-28.0$        | $1.50$        | $2.240$       |
| TS-N                 | $-27.0$        | $1.18$        | $2.051$       |
| TMo-O                | $-28.1$        | $1.15$        | $3.230$       |
| TS-O                 | $-27.0$        | $1.20$        | $2.000$       |
between NO molecular and MoS$\textsubscript{2}$ layer. The Mulliken/Hirshfeld charge of the NO molecule is 0.04 e and this positive charge indicates that the electrons transferred from NO molecule to monolayer MoS$\textsubscript{2}$. The large-scale orange region around NO molecule in charge density difference between NO and monolayer MoS$\textsubscript{2}$ (as shown in figure 3) further illustrates the electron depletion on NO molecule. Both the Mulliken/Hirshfeld charge and charge density difference suggest the charge-donor characteristics of NO molecule, which is consistent with Jianming Xue's result \cite{21}.

As for the case of NO-adsorbed on bilayer and trilayer MoS$\textsubscript{2}$ shown in figures 4 and 5, although the adsorption position, angle and height are different, the Mulliken/Hirshfeld charge and charge density difference show almost the same charge transfer character, indicating NO is also electron donor. The charge transfer between NO molecule and MoS$\textsubscript{2}$ layers can lead to the variation of its resistance when it is exposed to NO gas. For instance, charge accumulation in MoS$\textsubscript{2}$ layers increases the number of electrons and thus improves its charge carriers and weakens its resistance. Although NO adsorption on MoS$\textsubscript{2}$ layers shows physisorption characteristic, the significant charge transfer implies that MoS$\textsubscript{2}$ layers have a highest sensitivity towards NO gas. Moreover, the physisorption characteristic is beneficial for desorption, which could improve the recovery characteristics of gas sensors \cite{2}.

The band structures of pristine monolayer, bilayer and trilayer MoS$\textsubscript{2}$ are shown in figures 6(a), (d) and (g), respectively, from which we can obviously see that the band gap of MoS$\textsubscript{2}$ is decreased with the increase of the thickness. Moreover, the direct-to-indirect gap transition of MoS$\textsubscript{2}$ upon increase the thickness from single layer is also observed. Our findings are agreement with other first-principles calculations \cite{24}. Moreover, the band structures after NO adsorption are also shown in figure 6 for a comparison. Obviously, the outline of either the valence or conduction bands of MoS$\textsubscript{2}$ layers is not significantly influenced, which is consistent with their physisorption properties illustrated above. Nevertheless, NO adsorption induces an additional energy states at
Figure 4. NO adsorption on bilayer MoS₂. (a) Top and side views of optimized geometric structures. (b) Deformation electron density. (c) Charge density difference between NO and MoS₂ system.

Figure 5. NO adsorption on trilayer MoS₂. (a) Top and side views of optimized geometric structures. (b) Deformation electron density. (c) Charge density difference between NO and MoS₂ system.
about 0.5 eV, and it gives rise to a considerable upshift of the Fermi level as shown in figures 6(b), (e) and (h). Thus, the adsorption of NO gas results in n-type doping effect, which is consistent with the charge transfer analysis. Furthermore, the whole bands of MoS$_2$ shifted to low energy (occupied states) direction, reveals the reaction is exothermic. From the PDOS in figures 6(c), (f) and (i) we can obviously obtained two results. On the one hand, the DOS of MoS$_2$ with adsorption and no adsorption is similar, confirming the band structure results above. On the other hand, the additional states mainly induced by NO gas indicated by green curves in PDOS, which is beneficial for NO detection.

Due to the additional states in the band gap region near the bottom of the conduction band, NO adsorption will enhance the conductance of MoS$_2$ significantly, and then result in a noticeable change in the transport

Figure 6. Calculated band structures and corresponding PDOS of pure and NO-adsorbed (a)–(c) monolayer, (d)–(f) bilayer and (g)–(i) trilayer MoS$_2$. The Fermi energy is set at 0 eV.
properties of MoS$_2$. Here, we represent a semi-quantitative analysis about the variation of the electrical conductivity after adsorption. The electrical conductivity can be expressed by $\sigma = ne\mu$, in which $n$ and $\mu$ are carrier concentration and carrier mobility, respectively, and $e$ is electron charge. It has been proven that few-layer MoS$_2$ exhibits much higher electronic mobility compared with monolayer MoS$_2$.\cite{24}. In our calculation, the electronic properties of MoS$_2$ are almost consistent before and after NO adsorption. So, we only focus on the variation of the $\sigma$ after adsorption. The variation of band gap is directly related to the carrier concentration according to following relationship $n \propto \exp \left( -\frac{E_g}{k_\beta T} \right)$, where $k_\beta$ is the Boltzmann constant. Thus, the smaller the band gap is, the higher the carrier concentration is, and then the higher the conductivity is. After adsorption, band gaps (here, band gap indicates the energy difference between the highest occupied states and the lowest unoccupied states) of monolayer, bilayer and trilayer MoS$_2$ are 1.267, 0.696 and 0.577 eV, respectively, the corresponding reduction values are 0.503, 0.443 and 0.367 eV. The most considerable reduction of the band gap in monolayer MoS$_2$ would most significantly enhance the conductivity, compared with bilayer and trilayer MoS$_2$. However, the $n$ and $\mu$ are incompatible that $n$ and $\mu$ decreases and increases, respectively, with the thickness increases. According to our theoretical calculation, a few layers MoS$_2$ may have better NO detection performance than monolayer MoS$_2$. The specific number of layers with the best detection performance needs balance the $n$ and $\mu$, and deserves further exploration.

Conclusion

NO gas sensing plays an important role in environmental protection and human health. In the past decade, extensive research on 2D layered materials, especially TMDs, as a gas sensor was conducted due to its large surface to volume ratio, bandgap and cheapness properties. However, the relationships between NO gas-sensing properties and layer thickness have not been investigated. In our work, we systematically explored the NO adsorption behavior of the monolayer, bilayer and trilayer MoS$_2$. The results show that NO gas molecule is adsorbed on MoS$_2$ layers by van der Waals interaction under the analysis of adsorption energy, adsorption distance and deformation electron density. The change in the electronic conductivity and charge transfer induced by gas adsorption is responsible for the NO gas-sensing properties of MoS$_2$ layers. Our work shows that a few layers MoS$_2$ may have most excellent NO gas-sensing properties thus we don’t have to deliberately pursue monolayer MoS$_2$ in the experiment as a NO gas sensor.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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