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# **Enhanced Sensitivity of MoSe<sub>2</sub> Monolayer for Gas Adsorption Induced by Electric Field**

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## **Abstract**

According to recent studies, gas sensors based on MoSe<sub>2</sub> have better detection performance than graphene-based sensors, especially for N-based gas molecules, but the reason for that is not fully understood at the microscopic level. Here, we investigate the adsorption of CO, CO<sub>2</sub>, NH<sub>3</sub>, NO and NO<sub>2</sub> gas molecules on MoSe<sub>2</sub> monolayer by the density functional theory calculations. Our results reveal that indeed MoSe<sub>2</sub> monolayer is more sensitive to adsorption of N-containing gas molecules than C-containing, which can be attributed to the distinct charge transfer between the gas molecules and MoSe<sub>2</sub>. The conductance was further calculated using the nonequilibrium Green's function (NEGF) formalism. The reduced conductance was found for NH<sub>3</sub> and NO<sub>2</sub> adsorbed MoSe<sub>2</sub>, consistent with the high sensitivity of MoSe<sub>2</sub> for NH<sub>3</sub> and NO<sub>2</sub> molecules in the recent experiments. In addition, the adsorption sensitivity can significantly be improved by an external electric field, which implies the controllable gas detection by MoSe<sub>2</sub>. The magnetic moments of adsorbed NO and NO<sub>2</sub> molecules can also be effectively modulated by the field-sensitive charge transfer. Our results not only give microscopic explanations to the recent experiments, but also suggest using MoSe<sub>2</sub> as a promising material for controlled gas sensing.

Keywords: transition metal dichalcogenides, gas sensor, density functional theory calculations, electric field

## **Introduction**

Two-dimensional (2D) nanomaterials are ideal platforms for building nanoscale sensors due to their reduced dimensionality and excellent properties [1-8]. Recently,

2D transition metal dichalcogenides (TMDs) have attracted great interest as chemical sensors owing to their high carrier mobility [9-14], large surface-to-volume ratio [15-21], and rapid electrical response to the changes in the environments [22-24]. For instance, monolayer and multi-layer MoS<sub>2</sub> films have been found to be extremely sensitive to the environmental gas molecules, especially to NO, NO<sub>2</sub> and NH<sub>3</sub> [25-27]. MoSe<sub>2</sub> layer, one of the most important materials in the family of 2D TMDs, is expected to have excellent sensing performance due to similar electronic properties, and also the fact that the phototransistors based on MoSe<sub>2</sub> exhibited outstanding responsivity, high specific detectivity and fast response time [28, 29]. Indeed, recent experimental studies demonstrated that MoSe<sub>2</sub> sheets possess a competitive advantage over traditional graphene sensors [30]. In addition, Late *et al.* reported high-performance MoSe<sub>2</sub>-based NH<sub>3</sub> gas sensors with a detection limit down to 50 ppm [31]. More recently, a multilayer MoSe<sub>2</sub> gas sensor has exhibited ultra-high sensitivity ( $S \sim 2 \times 10^3$  for NO<sub>2</sub> at 300 ppm), owing to changes of the gap states near the valence band induced by the NO<sub>2</sub> adsorption [32]. However, the formation of these gap states has not been explained, and further verification is desired to carry out. These reports have stimulated exploration of MoSe<sub>2</sub> as a prospective sensing material.

In fact, the adsorption performance is mainly based on the charge transfer between the adsorption substrate and the gas molecules, which plays an important role in determining the performance of gas sensors. Therefore, effective control for electron transfer between gas molecules and sensing materials can modulate the sensitivity.

Calculations have demonstrated that the sensing properties of low dimensional materials, such as carbon nanotubes [33, 34], graphene [35, 36] and MoS<sub>2</sub> [37], are controllable by external electric field. For example, recent studies indicated that the adsorption of NO<sub>2</sub> based on Ga-doped graphene was effectively enhanced by the electric field, as manifested by the increase in adsorption energy [36]. Moreover, the charge transfer between the adsorbed molecule and MoS<sub>2</sub> can also be controlled by the external electric field [37]. In addition, the applied electric field could significantly enhance the CO gas sensitivity of the antimonene [38], which is beneficial for the application of CO gas sensor at room temperature. These studies suggested that the external electric field can dramatically change the affinity and electronic properties of the adsorption system. Therefore, it is expected that the electric field can effectively modulate the charge transfer between gas molecules and MoSe<sub>2</sub>, which inspired us to study if sensitivity of MoSe<sub>2</sub> for gas sensors can be improved by applying external electric field.

In this work, by means of systematic density functional theory (DFT) calculations, we examine the most stable adsorption configurations and also evaluate adsorption energy, charge transfer, and magnetic properties of gas molecules (CO, CO<sub>2</sub>, NH<sub>3</sub>, NO and NO<sub>2</sub>) on MoSe<sub>2</sub> monolayer. The results show that the adsorption energies of N-based gas molecules are larger than those for CO and CO<sub>2</sub> adsorption, which is related to the distinct charge transfer between the gas molecules and MoSe<sub>2</sub>. The reduced conductance was found for NH<sub>3</sub>, NO and NO<sub>2</sub> adsorbed MoSe<sub>2</sub>, which well explains

the high sensitivity of MoSe<sub>2</sub> to NH<sub>3</sub> and NO<sub>2</sub> adsorption as seen in recent experiments. In addition, the adsorption sensitivity can be significantly improved by an external electric field. The magnetic moments of adsorbed NO and NO<sub>2</sub> molecules can effectively be modulated by the charge transfer, which is sensitive to the applied electric field. Our results not only explain the recent experiments [31] at the atomistic level, but also suggest using MoSe<sub>2</sub> as a superior gas sensor.

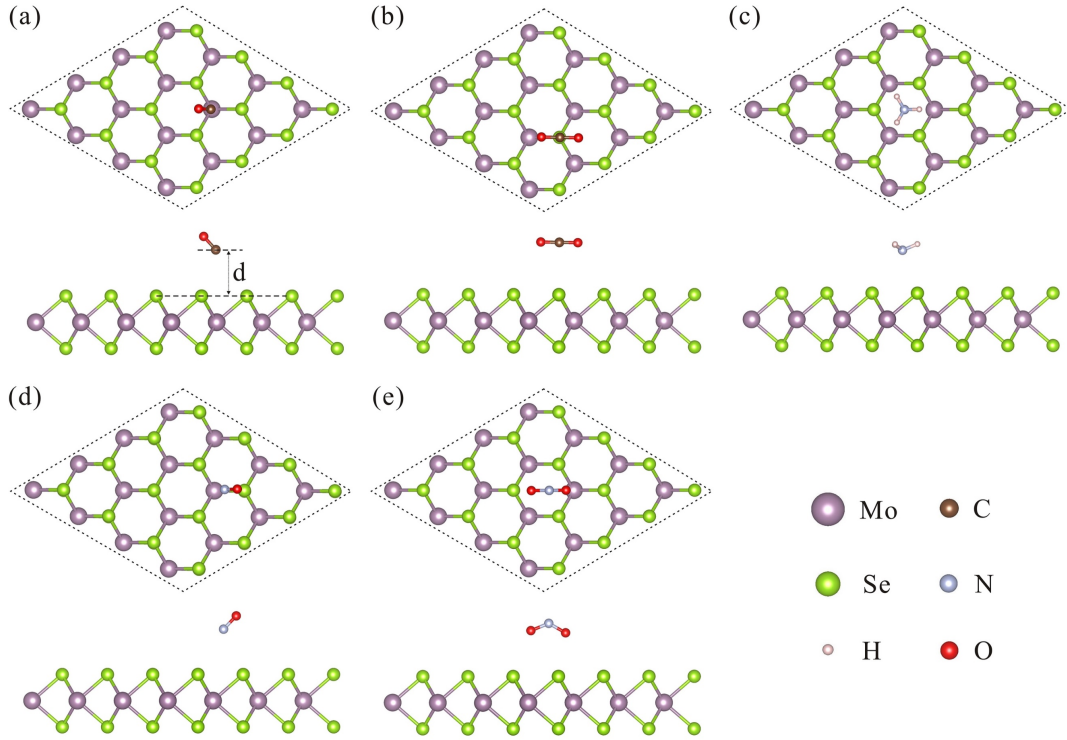
### Calculation details

Our calculations were carried out using the VASP package [39, 40] based on DFT. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) functional was used for the exchange and correlation interactions [41]. The projector-augmented-wave (PAW) method was employed to describe electron-ion interactions [42, 43]. Van der Waals corrections were included through Grimme's DFT-D2 method as implemented in VASP [44, 45]. The plane wave cutoff energy was set to 500 eV, because a higher value had little effect on the results. The structures were relaxed until the energy and the force on each atom were less than 10<sup>-5</sup> eV and 0.01 eV/Å, respectively. A k-point sampling of 9 × 9 × 1 and 19 × 19 × 1 were used for the structural relaxations and self-consistent calculations. The vacuum region of 15 Å was introduced to avoid interaction between periodic images of slabs. The charge transfer between gas molecules and MoSe<sub>2</sub> was calculated using Bader analysis [46]. Spin polarization was included in the calculations of the adsorption of paramagnetic molecules NO and NO<sub>2</sub>. The electronic transport properties were studied by the NEGF

method implemented in the TRANSIESTA package [47].

## Results and discussion

To model the absorption of CO, CO<sub>2</sub>, NH<sub>3</sub>, NO and NO<sub>2</sub> molecules on the surface of MoSe<sub>2</sub> monolayer, a 4 × 4 supercell of MoSe<sub>2</sub> was chosen. The optimized lattice constant of MoSe<sub>2</sub> monolayer was found to be 3.32 Å, consistent with the previous results [48,49]. In order to obtain the most stable adsorption configuration, the four different adsorption sites were considered (see Figure S1 in Supporting Information). (i) H site (on the top of a hexagon center), (ii) Tm (on the top of a Mo atom), (iii) Ts (on the top of a Se atom), (iv) B site (on the top of a Mo-Se bond). The top and side views of the most favorable configurations for CO, CO<sub>2</sub>, NH<sub>3</sub>, NO and NO<sub>2</sub> adsorbed on MoSe<sub>2</sub> are shown in Figure 1. For the CO and CO<sub>2</sub> molecules, the C atom is located at the Tm and Ts sites. The adsorption distance between the CO molecule and MoSe<sub>2</sub> (2.94 Å) is smaller than the value for CO<sub>2</sub> adsorption (3.30 Å). However, NH<sub>3</sub> and NO<sub>2</sub> molecules are located at the H site. The distances for NH<sub>3</sub> and NO<sub>2</sub> adsorption are 2.72 Å and 2.77 Å, respectively. In contrast, for NO, the molecule moves to the B site with the adsorption distance of 2.88 Å, as shown in Figure 2(a). The values indicate that upon adsorption the N-based gas molecules have the smaller distance as compared to those for CO and CO<sub>2</sub> molecules.

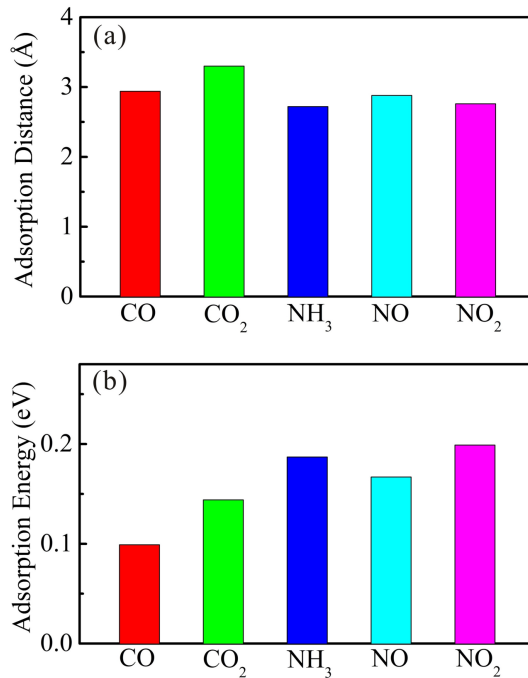


**Figure 1.** Top and side views of (a-e) the most favorable configurations of (a) CO, (b) CO<sub>2</sub>, (c) NH<sub>3</sub>, (d) NO, and (e) NO<sub>2</sub> adsorbed on MoSe<sub>2</sub> monolayer. The definition for the adsorption distance *d* is given in (a).

In order to get a quantitative description of the adsorption strength on MoSe<sub>2</sub> monolayer for different gas molecules, the adsorption energy was computed. The adsorption energy is defined as  $E_a = E_{\text{MoSe}_2} + E_{\text{molecule}} - E_{\text{total}}$ , where  $E_{\text{total}}$  is the total energy of MoSe<sub>2</sub> with an adsorbed molecule,  $E_{\text{MoSe}_2}$  and  $E_{\text{molecule}}$  are the total energies of the pristine MoSe<sub>2</sub> and isolated molecule, respectively. According to this definition, a more positive  $E_a$  value indicates a stronger adsorption. The calculated values of adsorption energy are displayed in Figure 2b. It is found that CO has the minimum adsorption energy of 0.099 eV, while NO<sub>2</sub> has the maximum adsorption energy of 0.199 eV. The adsorption energies of CO<sub>2</sub>, NO, and NH<sub>3</sub> are 0.144, 0.167,



and 0.187eV, respectively. The results show that the adsorption energies of N-based gases are larger than those for CO and CO<sub>2</sub> adsorption, which well correlates with the adsorption distances presented in Figure 2a. This indicates that MoSe<sub>2</sub> is more sensitive to adsorption of N-based gases, which is similar to MoS<sub>2</sub> and graphene that are sensitive to adsorption of N-based gases [14,26]. Among them, NH<sub>3</sub> and NO<sub>2</sub> have the highest adsorption energy, which explains the higher sensitivity to NH<sub>3</sub> and NO<sub>2</sub> adsorption on MoSe<sub>2</sub> as seen in the recent experiments [31, 32].

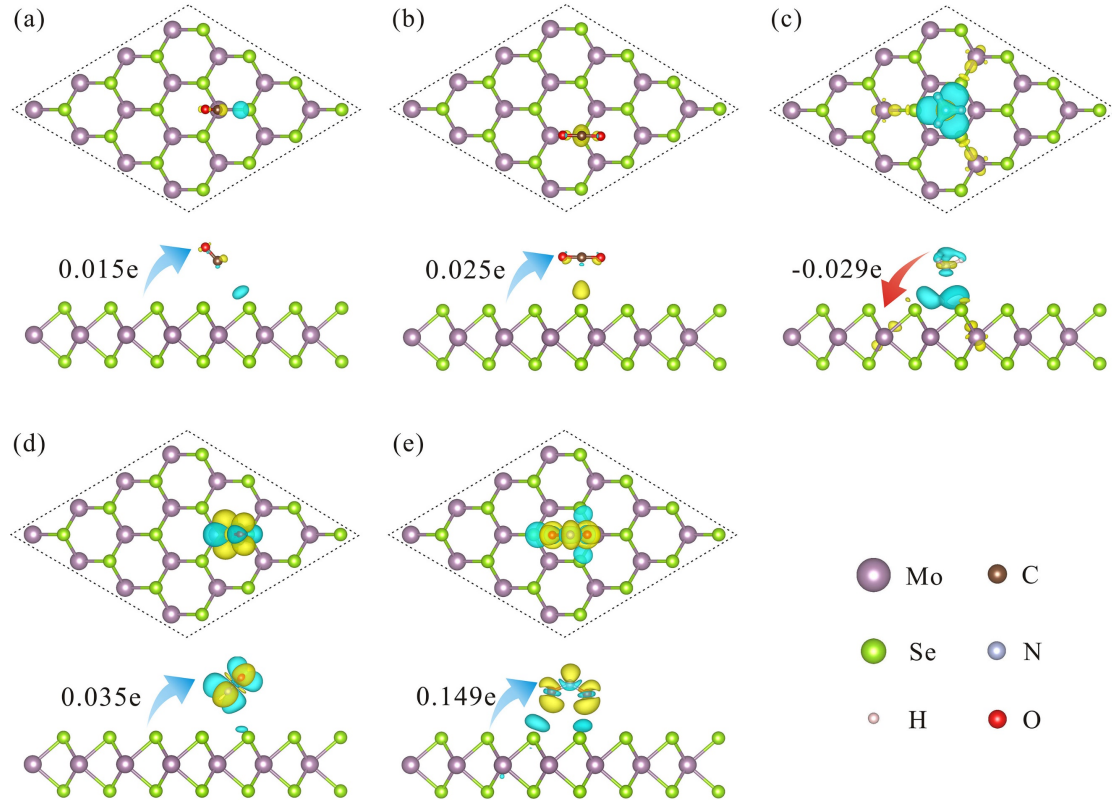


**Figure 2.** (a) Distance between the gas molecule and the MoSe<sub>2</sub> monolayer, defined as in Figure 1a. (b) Adsorption energy for CO, CO<sub>2</sub>, NH<sub>3</sub>, NO, and NO<sub>2</sub> on MoSe<sub>2</sub> monolayer.

Previous studies indicate that charge transfer plays an important role in the adsorption strength and the decrease in the resistance of MoS<sub>2</sub> [50]. Thus, we calculated the charge difference between the gas molecules and MoSe<sub>2</sub> monolayer (Figure 3), which is defined as  $\Delta\rho = \rho_{\text{gas/MoSe}_2} - \rho_{\text{gas}} - \rho_{\text{MoSe}_2}$ , where  $\rho_{\text{gas/MoSe}_2}$ ,  $\rho_{\text{gas}}$  and

$\rho_{\text{MoSe}_2}$  represent the charge density of the gas molecules adsorption system, the isolated gas molecule and the free MoSe<sub>2</sub> monolayer, respectively. Both the gas molecule and free MoSe<sub>2</sub> have the same coordination as that in the adsorbed configuration. To have a quantitative picture, Bader analysis was performed to extract the charge transfer amount induced by the gas adsorption. As shown in Figure 3a and 3b, for CO and CO<sub>2</sub> adsorption, the small amount of charge transfer (0.015 e and 0.025 e, respectively) is observed from MoSe<sub>2</sub> monolayer to the gas molecules, indicating the weak binding. However, for N-based gas molecules, larger charge transfer takes place, suggesting a stronger binding between the gas molecules and MoSe<sub>2</sub> monolayer. Especially for NO<sub>2</sub>, up to 0.149 e is transferred from MoSe<sub>2</sub> monolayer to the molecule (Figure 3e), which has the strongest binding. For NH<sub>3</sub> and NO adsorption in Figure 3c and d, the charge transfer (0.029 e and 0.035 e, respectively) is smaller than that for NO<sub>2</sub>, but still larger than those for CO and CO<sub>2</sub>. The comparison of the amount of the charge transfer and the adsorption energy (strength) presented in Figure 2b shows a clear correlation, which can help us to understand the mechanism for gas molecule adsorption on MoSe<sub>2</sub> monolayer. In addition, it is evident from Figure 3 that most molecules (such as CO, CO<sub>2</sub>, NO and NO<sub>2</sub>) are charge acceptors, whereas NH<sub>3</sub> behaves as a charge donor. The phenomenon is similar to the cases of gas adsorption on graphene and MoS<sub>2</sub> [37,51], where the gas molecules also behave as either charge acceptors or donors. For the n-type MoSe<sub>2</sub>, some electrons have already existed in the conduction band. Upon CO, CO<sub>2</sub>, NO and NO<sub>2</sub> adsorption, electron charge is transferred to the gas molecules from

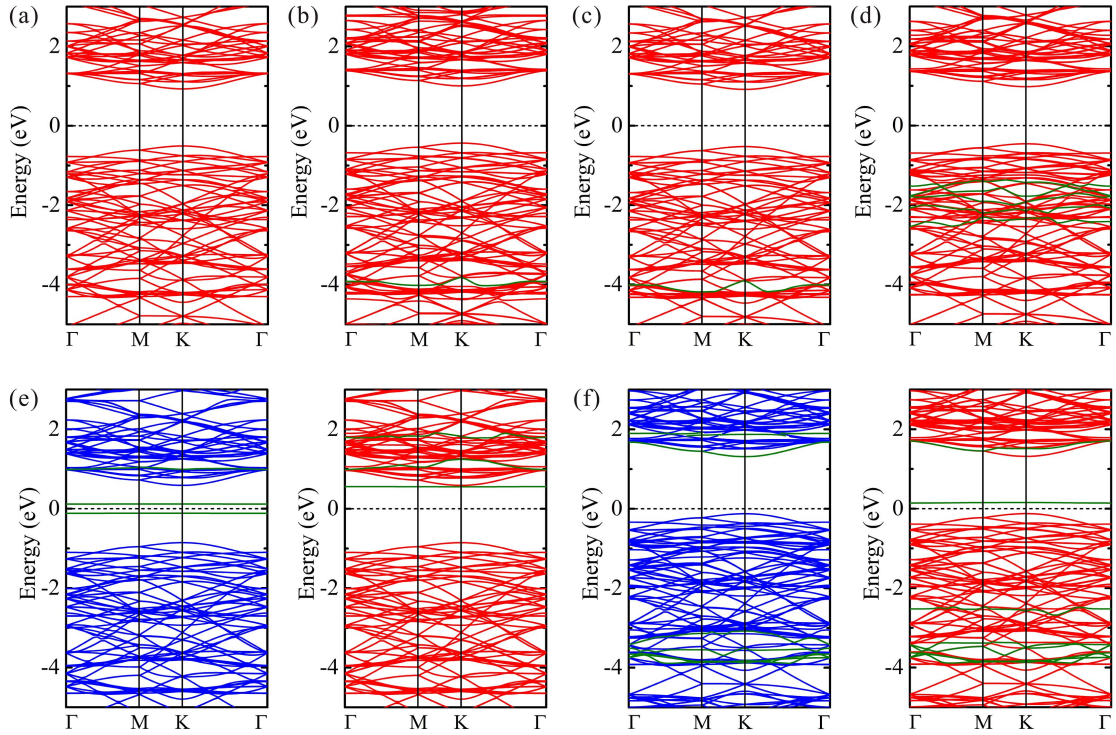
MoSe<sub>2</sub>, leading to an increased resistance and decreased current of MoSe<sub>2</sub>. Then, the mechanism of the MoSe<sub>2</sub>-FET gas sensor for NO<sub>2</sub> can be understood [32].



**Figure 3.** The charge difference between MoSe<sub>2</sub> monolayer and gas molecules for (a) CO, (b) CO<sub>2</sub>, (c) NH<sub>3</sub>, (d) NO and (e) NO<sub>2</sub>. The isosurface is taken at  $6.0 \times 10^{-4} \text{ e}/\text{\AA}^3$ . The electron accumulation (depletion) is indicated by yellow (blue) color. The direction (indicated by an arrow) and value of the charge transfer are shown.

Next, we examine the effects of gas adsorption on the electronic properties of MoSe<sub>2</sub> monolayer. Figure 4a shows the band structure of MoSe<sub>2</sub> monolayer, which has a direct bandgap of 1.44 eV, in accordance with previous reported results [48,49]. Figure 4b-d present the band structure of MoSe<sub>2</sub> monolayer with the adsorption of CO, CO<sub>2</sub> and NH<sub>3</sub>, as well as the projected band structure from the gas molecules. It is found that upon CO, CO<sub>2</sub> and NH<sub>3</sub> adsorption, neither the valence bands nor conduction band of

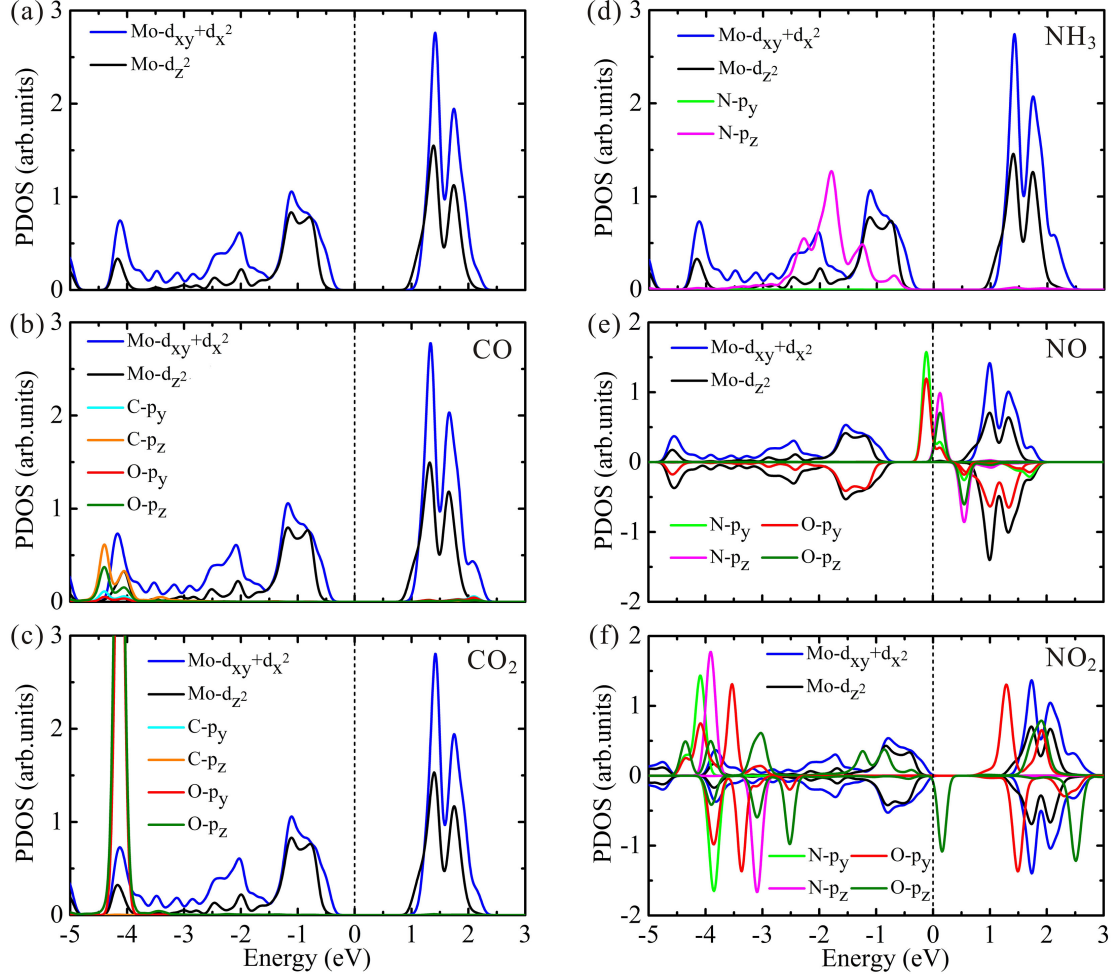
MoSe<sub>2</sub> monolayer is significantly influenced, as the impurity states induced by gas molecules located away from the Fermi level. Thus, CO, CO<sub>2</sub> and NH<sub>3</sub> adsorption does not modify the band structure near the Fermi level, and has no substantial influence on the electronic structure of MoSe<sub>2</sub> monolayer. On the other hand, the spin-polarized band structure of NO and NO<sub>2</sub> adsorbed MoSe<sub>2</sub> is displayed in Figure 4e and f. It is seen that for paramagnetic NO and NO<sub>2</sub> adsorption, some flat impurity states are clearly observed in the band gap of the host MoSe<sub>2</sub> monolayer. Specifically, NO introduces two spin-up states at -0.12, 0.12 eV and one spin-down state at 0.55 eV close to the Fermi level in the band gap (see Figure 4e). NO<sub>2</sub> introduces one spin-down state at 0.14 eV above the Fermi level in the band gap, given in Figure 4f. Our findings clearly explain the origin of the gap states in NO<sub>2</sub> adsorbed MoSe<sub>2</sub> in the recent experiments [32].



**Figure 4.** (a) The band structure of pristine MoSe<sub>2</sub>. Band structure of (b) CO, (c) CO<sub>2</sub>, (d) NH<sub>3</sub>, (e) NO and (f) NO<sub>2</sub> adsorbed on MoSe<sub>2</sub> monolayer. The blue and red lines denote spin-up and spin-

down channels, respectively. The olive lines represent the projected band structure of the adsorbed gas molecules.

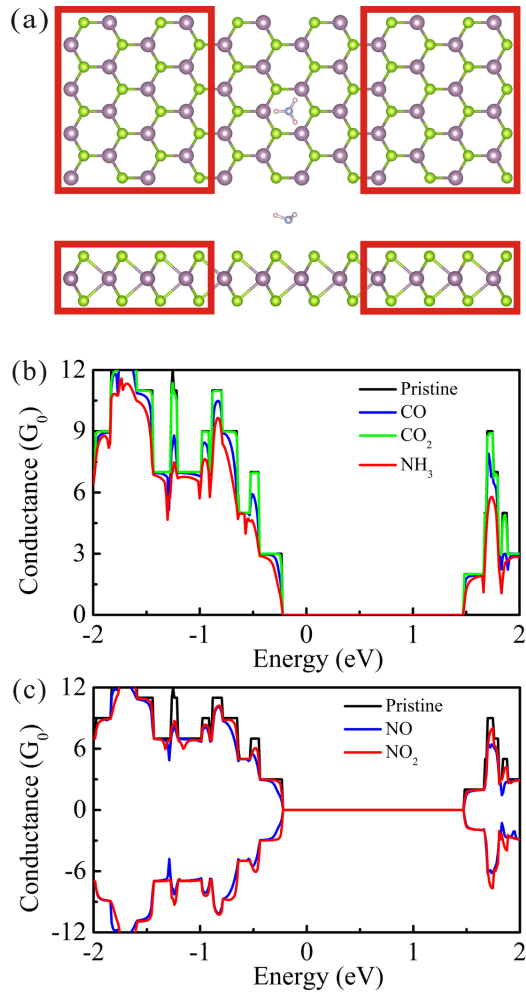
To further analyze the changes in electronic structure of MoSe<sub>2</sub> upon adsorption of the gas molecules, the projected density of states (PDOS) are calculated and presented in Figure 5. In the pristine MoSe<sub>2</sub> monolayer, the conduction band minimum is mainly described by Mo d<sub>z</sub><sup>2</sup> orbitals, while the valence band maximum is mostly contributed from Mo d<sub>xy</sub> and d<sub>x</sub><sup>2</sup> orbitals [48, 49]. For the CO and CO<sub>2</sub> adsorption, we did not observe noticeable changes around the Fermi level upon adsorption of the molecules, as indicated in Figure 5b and c, which is consistent with their small adsorption energies. Meanwhile, the adsorption of the NH<sub>3</sub> molecule induces some impurity states in the energy range around -2 eV, which leads to the hybridization of the N p<sub>z</sub> orbital with the d<sub>z</sub><sup>2</sup>, d<sub>x</sub><sup>2</sup> and d<sub>xy</sub> orbitals of the Mo atom. Overall, the adsorption of CO, CO<sub>2</sub> and NH<sub>3</sub> molecules does not have a noticeable effect on the DOS near the Fermi level. For the adsorption of NO, it can be seen from Figure 5e that the NO p<sub>y</sub> and p<sub>z</sub> orbitals dominate two DOS peaks around the Fermi level, which results in the flat impurity states for the spin-up electrons (see Figure 4e). Similarly, the adsorption of NO<sub>2</sub> produces a spin-down impurity state near the Fermi level, which is mainly composed of O p<sub>z</sub> orbitals, as shown in Figure 5f. It can be concluded that the adsorption of paramagnetic molecules NO and NO<sub>2</sub> induces the impurity states around the Fermi level, which have the obvious influence on the electronic structure of MoSe<sub>2</sub>, as manifested in their higher adsorption energy.



**Figure 5.** (a) PDOS of pristine MoSe<sub>2</sub>. PDOS of (b) CO, (c) CO<sub>2</sub>, (d) NH<sub>3</sub>, (e) NO and (f) NO<sub>2</sub> adsorbed on MoSe<sub>2</sub> monolayer.

Although the electronic properties of MoSe<sub>2</sub> are not significantly influenced by CO, CO<sub>2</sub>, and NH<sub>3</sub> adsorption, the resistivity of the system can be directly measured experimentally, which can be used as a signal for detecting gas molecules. In order to explore the resistivity change, we carried out the calculation of the conductance for MoSe<sub>2</sub> before and after the gas adsorption by the NEGF method. A two-probe system, where semi-infinite left and right electrode regions are in contact with the central scattering region, is used to calculate the electron transport properties, as shown in Figure 6a. We chose a  $4 \times 4$  supercell without gas adsorption for each of the left and

right electrodes, whereas the center scattering region was represented by a  $4 \times 4$  supercell with adsorbed gas molecules. Calculations for a  $4 \times 4$  central scattering region without gas adsorption were also done for comparison. For the nonmagnetic gas molecules adsorption ( $\text{CO}_2$ ), the conductance of the system was almost unchanged as compared to the pristine  $\text{MoSe}_2$ , while for  $\text{CO}$  and  $\text{NH}_3$  the conductance was detectably reduced, as shown in Figure 6b. The smaller conductance means a reduced current, which can be directly used to compare with the experimental measurements. Similarly, a reduction in the conductance for  $\text{NO}$  and  $\text{NO}_2$  adsorbed  $\text{MoSe}_2$  is also observed, Figure 6c, indicating the high sensitivity of  $\text{MoSe}_2$  sensor to N-based gas molecules. It should be noted that the significantly decreased conductance of  $\text{MoSe}_2$  with adsorbed  $\text{NH}_3$  and  $\text{NO}_2$  molecules is consistent with the high sensitivity of  $\text{MoSe}_2$  for  $\text{NH}_3$  and  $\text{NO}_2$  molecules reported in the recent experiments [31, 32].

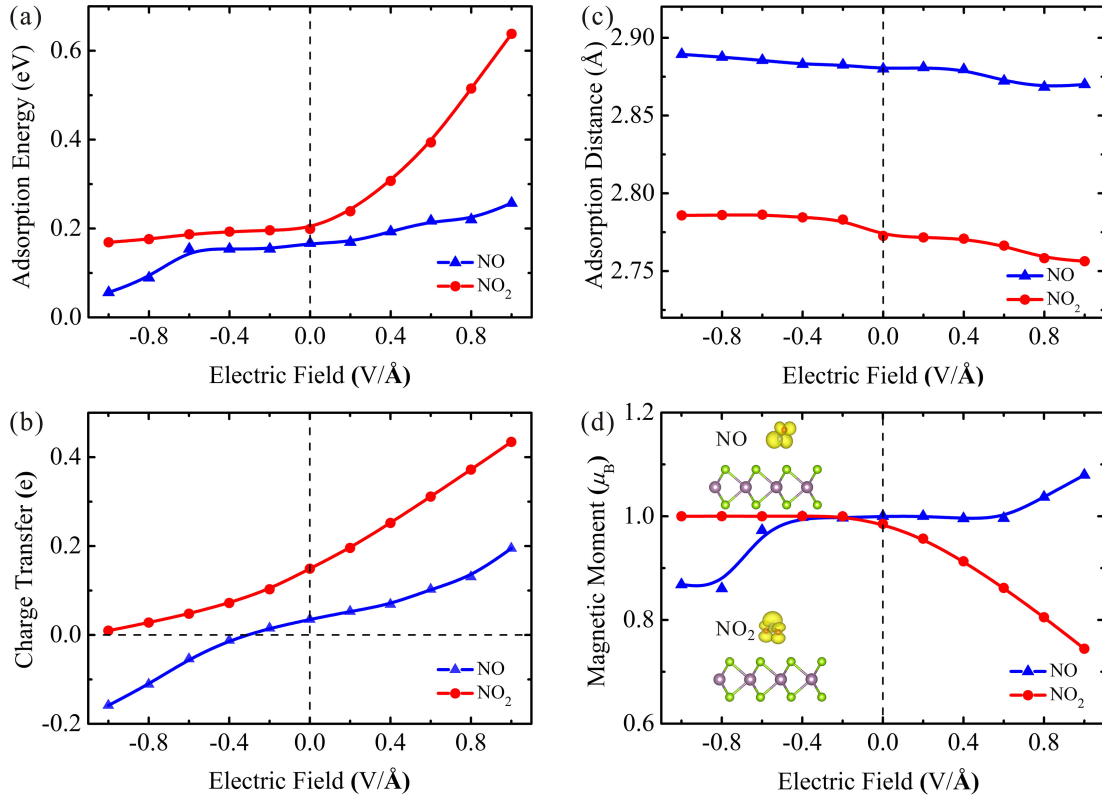


**Figure 6.** (a) Illustration of the two-probe systems where semi-infinite left and right electrode regions (red square region) are in contact with the central scattering region. The conductance of pristine MoSe<sub>2</sub> monolayer before and after (b) CO, CO<sub>2</sub> and NH<sub>3</sub>, (c) NO, NO<sub>2</sub> gas molecules adsorption.

Previous studies showed that the charge transfer upon adsorption can be tuned by perpendicular electric field, which plays an important role in determining the performance of MoSe<sub>2</sub> sensor. To explore the effect of the electric field on charge transfer, we applied an external vertical electric field across the plane of MoSe<sub>2</sub> monolayer. The positive direction of the electric field is defined from MoSe<sub>2</sub> monolayer to gas molecules. Taking the paramagnetic NO and NO<sub>2</sub> molecules as the representative



systems, we investigated the relationship between applied electric field with charge transfer, adsorption energy, adsorption distance as well as magnetic moment, displayed in Figure 7. It can be seen from Figure 7a that the adsorption energy is sensitive to the applied electric field. Along a positive electric field, the adsorption energy consistently increases with the increasing electric field. When a negative electric field is applied, the adsorption energy gradually decreases with the increasing negative electric field. In general, higher adsorption energy implies higher sensitivity for sensing application. The adsorption energy variation can be understood from the corresponding charge transfer and the adsorption distance, displayed in Figure 7b and c. Due to the strong electronegativity of N and O atoms, NO and NO<sub>2</sub> molecules are negatively charged. As compared to the case without electric field, there is additional electron transferred from MoSe<sub>2</sub> to NO and NO<sub>2</sub> at  $E = 1 \text{ V/\AA}$ , which will enhance the backdonation effect, as manifested in the enhanced adsorption energy and the reduced adsorption distance. On the other hand, the electrons transfer from NO and NO<sub>2</sub> to MoSe<sub>2</sub> as the increasing negative electric field, which weakens the backdonation effect and leads to smaller adsorption energy and larger adsorption distance. The same trend in the adsorption energy with charge transfer in the presence of the electric field was found upon adsorption of gas molecules on Ga-doped graphene [36]. Our results suggest that the sensitivity of MoSe<sub>2</sub> with adsorbed NO and NO<sub>2</sub> molecules can be significantly improved by applying an external vertical electric field.



**Figure 7.** Variation of (a) the adsorption energy, (b) the charge transfer, (c) the adsorption distance and (d) the magnetic moment as a function of electric field strength for NO and NO<sub>2</sub> adsorbed on MoSe<sub>2</sub> monolayer. The insets show the spatial spin density distribution on NO and NO<sub>2</sub> molecules.

At the same time, the adsorption of NO and NO<sub>2</sub> molecules can induce a magnetic moment of  $1.0 \mu_B$  and  $0.99 \mu_B$ , respectively. The spin density distribution shown in Figure 7d indicates that the spin-polarized electrons are mainly located on the NO and NO<sub>2</sub> molecules. Interestingly, the magnetic moment can be tuned by the applied electric field, as shown in Figure 7d. As for NO adsorption, the magnetic moment is almost unchanged in the low electric field strength. However, the magnetic moment reaches  $1.08 \mu_B$  or reduces to  $0.87 \mu_B$  at the electric field  $E = 1 \text{ V/\AA}$  and  $-1 \text{ V/\AA}$ , which can be attributed to the charge transfer. A Bader analysis indicates that there is  $0.035 \text{ e}$  electron transferred to NO at the absence of electric field, while NO accepts  $0.195 \text{ e}$  and donates

0.159 e at  $E = 1 \text{ V/\AA}$  and  $-1 \text{ V/\AA}$ , respectively. Similarly, for  $\text{NO}_2$  adsorption, the magnetic moment does not change too much due to charge transfer under a negative electric field, while it decreases to  $0.74 \mu_B$  at  $E = 1 \text{ V/\AA}$ . Thus, the magnetic moment of NO and  $\text{NO}_2$  gas molecules on  $\text{MoSe}_2$  can be effectively modulated by applying an external vertical electric field, which provides new strategy for constructing  $\text{MoSe}_2$ -based spin devices.

## Conclusions

In summary, using systematic DFT calculations, we have investigated the adsorption energy, charge transfer, electronic and magnetic properties of the gas molecules ( $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{NH}_3$ , NO and  $\text{NO}_2$ ) adsorbed on  $\text{MoSe}_2$  monolayer. The results show that the adsorption energies of N-based gas molecules are larger than those for CO and  $\text{CO}_2$  molecules, suggesting that  $\text{MoSe}_2$  is more sensitive to N-based gas molecules. Particularly,  $\text{NO}_2$  adsorption has the highest adsorption energy, which can help us to understand the mechanism of the  $\text{MoSe}_2$ -FET gas sensor operation upon  $\text{NO}_2$  adsorption. The reduced conductance was found for  $\text{NH}_3$ , NO and  $\text{NO}_2$  adsorbed  $\text{MoSe}_2$ , consistent with the high sensitivity of  $\text{MoSe}_2$  for  $\text{NH}_3$  and  $\text{NO}_2$  molecules as seen in the recent experiment. In addition, the adsorption sensitivity can be significantly improved by an external electric field. The magnetic moment of adsorbed NO and  $\text{NO}_2$  molecules can effectively be modulated by the charge transfer, which is sensitive to the applied electric field. Our results not only explain the recent experiments, but also suggest using  $\text{MoSe}_2$  as a superior gas sensor.

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