A DFT Study on the Adsorption of H$_2$S and SO$_2$ on Ni Doped MoS$_2$ Monolayer

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Abstract: In this paper, a Ni-doped MoS$_2$ monolayer (Ni-MoS$_2$) has been proposed as a novel gas adsorbent to be used in SF$_6$-insulated equipment. Based on the first-principles calculation, the adsorption properties of Ni-MoS$_2$ to SO$_2$ and H$_2$S molecules, the main decomposition components of SF$_6$ under a partial discharge (PD) condition have been studied. The adsorption energy, charge transfer, and structural parameters have been analyzed to find the most stable gas-adsorbed Ni-MoS$_2$. Furthermore, the density of states (DOS), projected density of states (PDOS), and electron density difference were employed to explore the interaction mechanism between SO$_2$, H$_2$S, and the Ni-MoS$_2$ surface. It is found that the H$_2$S molecule and SO$_2$ molecule interact with the Ni-MoS$_2$ surface by strong adsorption energy. Therefore, we conclude that the interaction between these two kinds of gases and the Ni-MoS$_2$ monolayer belongs to chemisorption, and the Ni-MoS$_2$ monolayer might be a promising gas adsorbent for the fault recovery of SF$_6$-insulated equipment. Additionally, we have to point out that all of the conclusions only considered the final adsorption energy, the barrier in the transition state has not been analyzed in this paper.

Keywords: SF$_6$ decomposition components; Ni-MoS$_2$ adsorbent; surface adsorption; DFT calculations

1. Introduction

Due to the excellent insulation and arc extinguishing properties of SF$_6$, it has obtained a wide application in gas-insulated equipment, such as gas-insulated switchgear (GIS), gas-insulated breaker (GIB), and gas-insulated transformer (GIT). In addition, SF$_6$-insulated equipment exhibits a great deal of advantages, such as a small occupied area requirement, little electromagnetic pollution, and high safety and reliability [1,2]. However, a certain amount of insulation defects inevitably occur in SF$_6$-insulated equipment during the long-term running process, which may lead to partial discharge (PD) and the decomposition from SF$_6$ to SF$_x$ under the operating voltage [3,4]. Simultaneously, the SF$_6$ gas-filled chamber inevitably contains trace amounts of impurities, such as H$_2$O and O$_2$ [5]. SF$_x$ will quickly react with the H$_2$O and O$_2$ into various decomposition components (such as H$_2$S, SO$_2$, SOF$_4$, SO$_2$F$_2$, SOF$_2$, HF, CF$_4$, and CO$_2$, etc.) [1,6–8]. These decomposition components can significantly accelerate the corrosion and aging process of the insulation medium, resulting in insulation failure. In order to ensure the running stability of SF$_6$-insulated equipment, the primary task is to maintain the purity of the filling gas, namely removing the decomposition components of SF$_6$ [9,10]. Considering all of the SF$_6$ decomposition components, H$_2$S, SO$_2$ gases, the main decomposition components under all types of PD conditions are the key removing target gases [11–13]. Thus, it is urgent to explore an effective adsorbent for H$_2$S and SO$_2$ removal.
Recently, along with the upsurge of research on graphene and other two-dimensional (2D) layered nanomaterials [14–16], the graphene-like MoS$_2$ monolayer, exhibiting good chemical stability and thermal stability, high specific surface area, and high surface activity, has attracted much research interest for various applications, including electrochemical lithium storage, solid lubrication, catalysis, and gas adsorbents [17–22]. Among them, the application of MoS$_2$ in gas adsorption has attracted much research attention in recent years. Liu et al. developed an ethanol gas sensor based on an indium oxide/molybdenum disulfide (In$_2$O$_3$/MoS$_2$) nanocomposite, and investigated its gas-sensing properties to ethanol gas [23]. Dongwei Ma et al. improved the sensing properties of MoS$_2$ to CO and NO by doping the MoS$_2$ monolayer with Au, Pt, Pd, and Ni, concluding that introducing appropriate dopants could be a feasible method to improve the gas sensing performance of MoS$_2$-based gas sensors [24]. The gas adsorption properties of common gases (CO, NO$_2$, H$_2$O, NH$_3$) on a pristine monolayer MoS$_2$ and a metal (V, Nb, Ta)-doped MoS$_2$ monolayer reported by Jia Zhu et al., indicated that metal doping can significantly improve the adsorption properties, chemical activity, and sensitivity of the MoS$_2$ monolayer [25].

On the one hand, metal atom doping provides a large number of free electrons, namely improving the electrical conductivity of the MoS$_2$ monolayer. On the other hand, the strong orbital hybridization between the metal atom and gas molecules enhances the gas adsorption capacity of the MoS$_2$ monolayer to gas molecules [24–27]. Herein, based on the first-principles calculation, we present an extensive theoretical investigation of the structure, total density of states (TDOS), and projected density of states (PDOS) of a Ni-doped MoS$_2$ monolayer. Additionally, its gas adsorption performance towards the typical SF$_6$ decomposition components H$_2$S and SO$_2$ has been systematically studied based on the analysis of structural parameters, TDOS, PDOS, and electron density difference. Furthermore, the gas adsorption mechanisms of the Ni-doped MoS$_2$ monolayer to H$_2$S and SO$_2$ was obtained based on the research above. In order to ensure the practicability of the adsorbent, the adsorption property of the Ni-MoS$_2$ monolayer towards SF$_6$ molecule has also been studied. In conclusion, the Ni-doped MoS$_2$ monolayer shows an ideal adsorption property to the target gases, signifying that it is a promising novel gas adsorbent used to ensure the running stability of SF$_6$-insulated equipment.

2. Computational Details

All calculations were performed based on the density functional theory (DFT) [28,29]. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) was chosen to calculate the geometry optimization with the energy convergence accuracy, maximum stress, and max displacement set to $1 \times 10^{-5}$ Ha, $2 \times 10^{-3}$ Ha/Å, and $5 \times 10^{-3}$ Ha, respectively [30,31]. The effect of spin-polarization was ignored in this paper, and Grimme dispersion correction has been introduced to describe the weak interactions, like van der Waals force. The double numerical plus polarization (DNP) was chosen as the basis set, the density functional semi-core pseudopotential (DSPP) was applied in core treatment, and the Monkhorst-pack k point mesh of $5 \times 5 \times 1$ was employed [32,33]. The self-consistent (SCF) field tolerance was set to $1 \times 10^{-6}$ Ha, and the DIIS size was set to 6 to speed up the convergence of SCF [34].

A $4 \times 4 \times 1$ MoS$_2$ monolayer supercell with a 20 Å vacuum slab, including 32 S atoms and 16 Mo atoms, was built in order to avoid the interaction between the adjacent cells. The optimized lattice constant of MoS$_2$ is calculated to be 3.180 Å, which is in good agreement with other theoretical calculation results [35]. One Ni atom was placed on the top site of the Mo atom at the center of the $4 \times 4 \times 1$ MoS$_2$ monolayer supercell, bonding with three S atoms.

The adsorption energy ($E_{\text{ads}}$) was calculated by Equation (1) [36]:

$$E_{\text{ads}} = E_{\text{Ni-MoS}_2/gas} - E_{\text{Ni-MoS}_2} - E_{\text{gas}}$$

where $E_{\text{Ni-MoS}_2/gas}$ is the total energy of the gas adsorbed Ni-MoS$_2$, while $E_{\text{Ni-MoS}_2}$ and $E_{\text{gas}}$ represent the total energy of the Ni-MoS$_2$ monolayer and the total energy of free gas molecule, respectively.
The more negative $E_{ads}$ obtained after geometry optimization, the easier for the free gas molecule to be adsorbed on the Ni-MoS$_2$ monolayer surface, indicating the adsorption system is more stable.

In addition, the charge transfer ($Q_t$) between the gas molecule and Ni-MoS$_2$ monolayer was calculated by Equation (2):

$$Q_t = Q_a - Q_b$$  \hspace{1cm} (2)

where $Q_a$ and $Q_b$ represent the amounts of carried charge of the gas molecules after and before gas adsorption, which were calculated by electron population analysis [37]. It is worth putting out that the value of $Q_b$ is always 0 $e$ in this paper. According to the definition, if $Q_t$ is positive, the electrons transfer from gas molecule to the Ni-MoS$_2$ monolayer. Additionally, the density of states (DOS) was calculated to analyze the interaction mechanism between gas molecules and the Ni-MoS$_2$ monolayer [38].

3. Results and Discussion

3.1. Structures and Electronic Properties of H$_2$S, SO$_2$ and the Ni-MoS$_2$ Monolayer

Firstly, the adsorption property of the Ni atom on the MoS$_2$ monolayer was discussed according to the adsorption energy analysis and population analysis. The adsorption energy ($E_{ads}$) of Ni atom on MoS$_2$ monolayer was defined in the Equation (3):

$$E_{ads} = E_{Ni-MoS_2} - E_{Ni} - E_{MoS_2}$$  \hspace{1cm} (3)

The negative $E_{ads}$ in Equation (3) indicates that the binding process is exothermic. As the most stable doping position of Ni on MoS$_2$ monolayer is the top site of the Mo atom according to previous studies [24], therefore, only the structure of Ni-MoS$_2$ with Ni doping on the top site of the Mo is discussed in this paper.

As shown in Figure 1, The Ni atom above the Mo3 atom bonds with other three surrounding S atoms with a length of 2.121 Å, and there is no chemical bond between the doped Ni atom and the Mo3 atom because of the long distance between them (2.596 Å). The bond angle of the Mo1-S1-Mo2 near the Ni atom (81.3°) has slightly changed compared with that of the MoS$_2$ monolayer without doping (82.0°), indicating that the doped Ni atoms have a strong interaction with the initial MoS$_2$ monolayer structure, and the doping structure could be quite stable. Moreover, the large binding energy (3.495 eV) further confirmed the conclusion above. In addition, the charge transfer from the Ni atom to the MoS$_2$ monolayer is 0.021 $e$.

To further analyze the structural properties of Ni-MoS$_2$ monolayer, the total density of states (TDOS) and projected density of states (PDOS) have been calculated as shown in Figure 2. For TDOS distribution, the electron distribution of the Ni-MoS$_2$ monolayer around the Fermi level has slightly increased compared with that of the MoS$_2$ monolayer, implying that the doping of the Ni atom has enhanced the metallic property of the MoS$_2$ monolayer. As a result, the doped Ni atom acts as the active site for building interaction between the Ni-MoS$_2$ monolayer and the target gas molecules. For PDOS distribution, the peaks of Ni-3d orbital and S-3p orbital overlap at $-5.5$ eV, $-4.5$ eV, $-3.5$ eV, $-2.5$ eV, and 2.0 eV, indicating that the S-3p orbital strongly hybridize with the Ni-3d orbital. Therefore, the Ni atom adsorbs on the surface of MoS$_2$ monolayer by a stable structure.

The structures of the gas molecules are exhibited in Figure 3, and its specific structural parameters of the gas molecules are listed in Table 1. Additionally, the carried charge of S and O atom in the SO$_2$ are 0.453 $e$ and $-0.227$ $e$, respectively. The H atom in the H$_2$S has a positive charge of 0.174 $e$, and the S atom has a negative charge of 0.348 $e$. For the SF$_6$ molecule, the charge of the S atom is calculated to be 1.194 $e$, and the F atom is $-0.199$ $e$. These results are in agreement with the other theoretical calculation reports [39].
Figure 1. The structure of Ni-MoS$_2$ monolayer: (a) top view; (b) side view.

Figure 2. (a) The TDOS of Ni-MoS$_2$; (b) the PDOS of Ni-MoS$_2$, the dashed lines represent the Fermi level.

Figure 3. The molecular structures of gas molecules: (a) H$_2$S; (b) SO$_2$; (c) SF$_6$. 
3.2. Adsorption of H$_2$S Gas on the Ni-MoS$_2$ Monolayer

To analyze the adsorption properties of Ni-MoS$_2$ monolayer to the target gas molecules, various initial approaching sites of H$_2$S to the Ni-MoS$_2$ monolayer were calculated in order to obtain the most stable adsorption structure. After optimization, only one typical adsorption structure was received, as shown in Figure 4 in the top view and side view, and its $E_{\text{ads}}$, $Q_t$, and specific structure parameters are shown in Table 2.

![Figure 4](image_url)

**Figure 4.** The configuration of the H$_2$S-adsorbed Ni-MoS$_2$ monolayer: (a) top view; (b) side view.

| Configuration | $E_{\text{ads}}$ (eV) | $Q_t$ (e) | $d_{\text{H1-S}}$ (Å) | $d_{\text{Ni-H2S}}$ (Å) | $\angle \text{H1-S-H2}$ (°) |
|---------------|-----------------|--------|----------------|----------------|--------------------|
| Figure 4      | −1.319          | 0.254  | 1.362          | 2.205          | 91.5               |

For adsorption system with structure shown in Figure 4a,b, a Ni-S bond with a length of 2.205 Å forms in the adsorption process, and the amount of the electrons transferred from the H$_2$S molecule to Ni-MoS$_2$ monolayer is up to 0.254 e, which means the S-Ni bond is not easy to break. However, the structure of the H$_2$S has slightly changed after adsorption. The length of the H-S bond increases to 1.362 Å, the angle of the H1-S-H2 turned into 91.5°. The $E_{\text{ads}}$ of H$_2$S on the Ni-MoS$_2$ monolayer is −1.319 eV, which is large enough to completely adsorb H$_2$S. Though barrier exists in the transition state, but the change of the structure of H$_2$S is not obvious, therefore, we conclude that the large $E_{\text{ads}}$ can provide the energy to cross over the barrier. As a result, from the amount of electrons transfer and $E_{\text{ads}}$, we conclude that the structure is the most stable structure for H$_2$S adsorption.

Figure 5 presents the TDOS and PDOS of Ni-MoS$_2$ monolayer before and after H$_2$S molecule adsorption. The TDOS after H$_2$S molecule adsorption shows a significant increase near −7 eV and −15 eV. Due to the main contribution of the outer orbitals of interacted atom in the adsorption process, only the PDOS of the S-3p and Ni-3d was discussed. The PDOS analysis shows that the S-3p orbitals overlaps with the Ni-3d orbitals in the range from −6 eV to 0 eV, and the overlapped peaks of these two orbitals appear at about −5 eV, −4 eV, −3.5 eV, −2.5 eV, and 1.5 eV. The wide range of overlap fully verifies the strong hybridization between these two orbitals. The analysis of TDOS and PDOS furtherly confirms the strong interaction between H$_2$S and Ni-MoS$_2$ monolayer, and its structure is quite stable.

### Table 1. The structural parameters of H$_2$S, SO$_2$, and SF$_6$.

| Gas Molecule | Bond Angle (°) | Bond Length (Å) |
|--------------|----------------|-----------------|
|              | Type | Angle | Type | Length |
| SO$_2$       | O1-S-O2   | 120.2   | O1-S | 1.480 |
| H$_2$S       | H1-S-H2   | 91.2    | H1-S | 1.356 |
| SF$_6$       | F1-S-F2   | 90.0    | F1-S | 1.616 |
Figure 5. (a) The TDOS of Ni-MoS$_2$ with and without H$_2$S adsorption; (b) the PDOS of main interacted atoms, the dashed lines represent the Fermi level.

Figure 6 shows the electron density difference of the H$_2$S adsorbed Ni-MoS$_2$ monolayer from different side views, where the increase and decrease of the electron density are represented by the red and blue region, respectively. From the electron density difference, it is intuitive to analyze the charge distribution after the gas adsorption. It can be found that both of the H atoms receive electrons, while the electron density near the S atom and Ni atom suffer a reduction and increase, respectively, which is in agreement with the conclusion that the H$_2$S molecule transfers quite a number of electrons to the monolayer. It is also interesting to notice that the electron density near the Mo atom below the Ni atom suffers an obvious reduction, and we assume that the electrons from the Mo atom made a contribution to the increase of the electron density surrounding H atoms. Therefore, the H$_2$S molecule brings a dramatic change of electron density to the Ni-MoS$_2$ monolayer.

In conclusion, considering the structure parameters, charge transfer, adsorption energy, DOS, and electron density difference of H$_2$S adsorbed Ni-MoS$_2$ monolayer, it is obvious that the interaction between the H$_2$S and the Ni-MoS$_2$ monolayer belongs to chemisorption. In consequence, this configuration is the most stable adsorption structure for H$_2$S adsorption on a Ni-MoS$_2$ monolayer. The Ni-MoS$_2$ monolayer shows an outstanding adsorption property to H$_2$S molecules.

3.3. Adsorption of SO$_2$ Gas on a Ni-MoS$_2$ Monolayer.

For the adsorption of SO$_2$ gas, the gas molecule is initially placed at various sites to approach the surface of the Ni-MoS$_2$ monolayer. Three typical adsorption structures were obtained after geometric optimization, as shown in Figure 7. Table 3 shows the structural parameters of these configurations.
Table 3. The structural parameters of adsorption configurations of the SO$_2$-adsorbed Ni-MoS$_2$ monolayer.

| Configuration | $E_{\text{ads}}$ (eV) | $Q_t$ ($\mu$) | $d_{\text{O1-S}}$ (Å) | $d_{\text{O2-S}}$ (Å) | $d_{\text{Ni-S}}$ (Å) | $d_{\text{Ni-O1}}$ (Å) | $\angle\text{O1-S-O2}$ (°) |
|---------------|------------------|----------------|-----------------|----------------|----------------|----------------|----------------|
| M1            | $-0.823$         | $-0.094$       | 1.543           | 1.489          | -              | 1.903          | 115.2          |
| M2            | $-1.382$         | $-0.016$       | 1.481           | 1.481          | 2.059          | -              | 119.2          |
| M3            | $-1.327$         | $-0.206$       | 1.575           | 1.494          | 2.238          | 1.948          | 116.6          |

Figure 7a,b shows the top view and side view of the M1 system. It can be seen that the SO$_2$ molecule adsorbs on the Ni-MoS$_2$ monolayer through the Ni-O1 bond, and the length of the Ni-O1 bond is 1.903 Å. The O1-S bond of SO$_2$ adsorbed on the monolayer is 1.543 Å, which slightly longer than that of a free SO$_2$ molecule (1.480 Å). The angle of the O1-S-O2 has decreased 5°. Thus, the structure of the SO$_2$ molecule changes very little during the adsorption process. The $E_{\text{ads}}$ of the M1 system is calculated to be $-0.823$ eV, 0.094 $\mu$ transfers from the Ni-MoS$_2$ monolayer to the SO$_2$ molecule. Due to
the strong interaction between \( \text{SO}_2 \) and the Ni-MoS\(_2\) monolayer, the adsorption of the M1 system belongs to chemisorption.

The top view and side view of the M2 system are given in Figure 7c,d, the \( \text{SO}_2 \) molecule adsorbs on the monolayer with a Ni-S bond length of 2.059 Å. From the structural parameters in Table 3, it is found that the structure of the \( \text{SO}_2 \) molecule changes little after adsorption. The \( E_{\text{ads}} \) of the M2 system has increased to \(-1.382\) eV compared to that in the M1 system, which manifests the stability of the M2 system. In addition, only \( 0.015 \) e transfers from the \( \text{SO}_2 \) molecule to the Ni-MoS\(_2\) monolayer in the M2 system, and the charge transfers from the S atom, O1 atom, and O2 atom are \( 0.050 \) e, \(-0.033 \) e, and \(-0.033 \) e, respectively.

The top view and side view of the M3 system are given in Figure 7e,f, the O1 atom and S atom are trapped by the Ni-MoS\(_2\) monolayer with bond lengths of 1.948 Å (Ni-O1) and 2.258 Å (Ni-S). Due to the strong interaction of the Ni-O1 bond and Ni-S bond, the \( Q_1 \) of the M3 system is calculated to be \(-0.206 \) e, which is distinctly larger than that in the M1 and M2 system. From the structural parameters in Table 3, the bond distance and angle in the \( \text{SO}_2 \) molecule insignificantly change after adsorption. The \( E_{\text{ads}} \) of M3 exhibited in Table 3 is \(-1.327\) eV, which is slightly smaller than that in the M2 system. Above all, according to the large amount of \( E_{\text{ads}} \) and charge transfer between the \( \text{SO}_2 \) molecule and the M2 system, chemisorption of Ni-MoS\(_2\) monolayer to \( \text{SO}_2 \) can be concluded. Although the \( E_{\text{ads}} \) of M3 system is very close to that of the M2 system, these two new built bonds between the \( \text{SO}_2 \) molecule and Ni atom in M3 system means a higher barrier during the adsorption process. Therefore, the M2 system is the most stable configuration. To further verify the conclusion, the DOS and the electron density difference are intensively discussed below.

Figure 8a shows the TDOS of the M2 system. It is obvious that a small change occurs in TDOS around the area of \(-20\) eV, \(-10.5\) eV, \(-7\) eV, \(-3\) eV, and \(-1\) eV for the \( \text{SO}_2 \)-adsorbed Ni-MoS\(_2\) monolayer. Similarly, as the adsorption process mainly contributed by of the outmost orbitals of atoms, only the PDOS of the S-3p and Ni-3d are discussed, as shown in Figure 8b. According to the PDOS results, the peaks of S-3p orbital and the Ni-3d orbital overlap at \(-5.5\) eV, \(-4\) eV, \(-2\) eV, and \(2\) eV, suggesting that the interaction between \( \text{SO}_2 \) and Ni-MoS\(_2\) monolayer is strong chemisorption, and its electronic structures are relatively active. Considering the large contribution of the S-3p orbital in the adsorption process, we confirm that the \( \text{SO}_2 \) adsorption structure in the M2 system is very stable.

![Figure 8](image_url)

**Figure 8.** (a) The TDOS of Ni-MoS\(_2\) with and without \( \text{SO}_2 \) adsorption; (b) the PDOS of the main interacted atoms in the M2 system. The dashed lines represent the Fermi level.

With respect to the electron density difference in the M2 system, shown in Figure 9, the increase and decrease of the electron density are represented by the red and blue regions, respectively. It is found that two O atoms in \( \text{SO}_2 \) receive electrons, and the electron density near the S atom decreases during the adsorption. In generally, the \( \text{SO}_2 \) molecule acts as an electron acceptor according to the electron density distribution.
3.4. Adsorption of SF$_6$ Gas on the Ni-MoS$_2$ Monolayer

In order to ensure the practicability of the Ni-MoS$_2$ adsorbent, the adsorption property of the Ni-MoS$_2$ monolayer towards the SF$_6$ molecule has also been studied, as SF$_6$ will always be the largest part of components in SF$_6$-insulated equipment. Various initial approaching sites of SF$_6$ to the Ni-MoS$_2$ monolayer were calculated in order to obtain the most stable adsorption structure. Two adsorption structures were received after geometric optimization, as shown in Figure 10 with different views. In addition, its adsorption energy, charge transfer, and other specific structural parameters are given in Table 4.

Figure 9. Electron density difference of the SO$_2$-adsorbed Ni-MoS$_2$ monolayer in the M2 system.

Figure 10. The adsorption configurations of the SF$_6$ adsorbed Ni-MoS$_2$ monolayer. (a,b) top and side view of M1; (c,d) top and side view of M2.
Table 4. The structural parameters of adsorption configurations of the SF$_6$ adsorbed Ni-MoS$_2$ monolayer.

| Configuration | $E_{\text{ads}}$ (eV) | $Q_t$ (e) | $d_{\text{Ni-F1}}$ (Å) | $d_{\text{Ni-F2}}$ (Å) | $d_{\text{F1-S}}$ (Å) | $d_{\text{F2-S}}$ (Å) | $\angle \text{F1-S-F2}$ (°) |
|---------------|----------------------|-----------|------------------------|------------------------|----------------------|----------------------|---------------------------|
| M1            | −0.174               | −0.445    | 1.875                  | 3.560                  | 1.796                | 1.684                | 89.3                      |
| M2            | −0.181               | −0.454    | 1.871                  | 3.511                  | 1.851                | 1.685                | 89.0                      |

As the parameters show in the Table 4, the $E_{\text{ads}}$ is only −0.174 eV for M1, and 0.181 eV for M2. $Q_t$ is −0.445 e and −0.454 e for the M1 and M2 structures, respectively. Though the $d_{\text{F1-S}}$ of SF$_6$ suffers a very small increase compared with that of free SF$_6$ molecule, it is still difficult to break its chemical bonds by the weak adsorption energy. Therefore, the SF$_6$ molecule interacts with Ni-MoS$_2$ monolayer by physisorption. Once H$_2$S and SO$_2$ decomposition components occur in SF$_6$-insulated equipment, H$_2$S and SO$_2$ quickly fill the role of the adsorption of SF$_6$ because of its strong adsorption energy of H$_2$S and SO$_2$. Additionally, the repulsion between gas molecules will block the interaction between the SF$_6$ molecule and Ni-MoS$_2$ monolayer. As a result, the Ni-MoS$_2$ monolayer can be a good adsorbent to H$_2$S and SO$_2$ in a SF$_6$ atmosphere.

4. Conclusions

In this study, a Ni-MoS$_2$ monolayer material has been proposed as a potential adsorbent to remove the typical decomposition components of SF$_6$ under partial electric discharge: H$_2$S and SO$_2$. All of the calculations performed with respect to density functional theory analysis and all of the conclusions only considered the final adsorption energy; the barrier in transition state has not been analyzed in this paper. Various adsorption models of H$_2$S and SO$_2$ molecules on the Ni-MoS$_2$ monolayer were built to find the most stable adsorption structure by analyzing the adsorption energy, charge transfer, and other structural parameters. To further analyze the interaction mechanism, the DOS, PDOS and electron density difference were presented and analyzed. We concluded that H$_2$S and SO$_2$ tend to adsorb on the surface of Ni-MoS$_2$ monolayer by chemisorption, and the adsorption energy of the H$_2$S and SO$_2$ is up to −1.319 eV and −1.382 eV, respectively, indicating that the interaction between these two kinds of gases and the Ni-MoS$_2$ monolayer is pretty strong. Additionally, the weak physisorption between SF$_6$ and the Ni-MoS$_2$ monolayer provides the basis for selectively adsorbing H$_2$S and SO$_2$ from the SF$_6$ atmosphere. Therefore, the Ni-MoS$_2$ monolayer might be a promising gas adsorbent to remove these two typical decomposition components of SF$_6$, which plays a key role in enhancing the running stability of SF$_6$-insulated equipment.

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