**Gas-Sensing Properties of B/N-Modified SnS\(_2\) Monolayer to Greenhouse Gases (NH\(_3\), Cl\(_2\), and C\(_2\)H\(_2\))**

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**Abstract:** The adsorption capacity of intrinsic SnS\(_2\) to NH\(_3\), Cl\(_2\), and C\(_2\)H\(_2\) is very weak. However, non-metallic elements B and N have strong chemical activity, which can significantly improve the conductivity and gas sensitivity of SnS\(_2\). Based on density functional theory, SnS\(_2\) was modified with B and N atoms to analyze its adsorption mechanism and gas sensitivity for NH\(_3\), Cl\(_2\), and C\(_2\)H\(_2\) gases. The optimal structure, adsorption energy, state density and frontier molecular orbital theory are analyzed, and the results are in good agreement with the experimental results. The results show that the adsorption of gas molecules is exothermic and spontaneous. Only the adsorption of NH\(_3\) and Cl\(_2\) on B-SnS\(_2\) belongs to chemical adsorption, whereas other gas adsorption systems belong to physical adsorption. Moderate adsorption distance, large adsorption energy, charge transfer and frontier molecular orbital analysis show that gas adsorption leads to the change of the conductivity of the modified SnS\(_2\) system. The adsorption capacity of B-SnS\(_2\) to these gases is Cl\(_2\) > NH\(_3\) > C\(_2\)H\(_2\). The adsorption capacity of N-SnS\(_2\) is NH\(_3\) > C\(_2\)H\(_2\) > Cl\(_2\). Therefore, according to different conductivity changes, B-SnS\(_2\) and N-SnS\(_2\) materials can be developed for greenhouse gas detection of gas sensors.

**Keywords:** greenhouse gases; SnS\(_2\); surface modification; adsorption; DFT

1. Introduction

With the continuous progress of society, the traditional agricultural production mode has been unable to meet the needs of modern civilization, which prompts the development of greenhouse planting [1–3]. It can be applied in the plateau, deep mountains, deserts, and other unique environments for agricultural production [4,5]. The illuminance, temperature, and humidity, and gas composition are the critical environmental parameters that affect planting growth [6]. In the actual cultivation process, the illuminance, temperature, and humidity can be easily regulated by changing the ceiling coverage and ventilation rate [7,8]. It is urgent to accurately monitor the greenhouse’s characteristic gas composition in the greenhouse online. Due to the half-open structure of the greenhouse, the accumulated gases are mainly NH\(_3\), Cl\(_2\), and C\(_2\)H\(_2\) [9,10].

Two-dimensional SnS\(_2\) is widely used in the gas sensor industry because of its large specific surface area and pore structure [11]. Compared with carbon nanotubes, SnS\(_2\) is more resistant to oxidation and more stable at high temperatures, making SnS\(_2\) more suitable for gas-sensing detection than carbon nanotubes [12]. It has become one of the most promising materials used in high-temperature and high-pressure environments [13]. However, pristine SnS\(_2\) has a limited reaction to gases, such as C\(_2\)H\(_4\), C\(_2\)H\(_2\), and NH\(_3\) [14]. Studies showed that non-metals modification could improve the gas detection accuracy and adsorption capacity of gas-sensing materials by regulating their energy gap and conductivity upon gas adsorption [15]. B and N are the most widely used modified non-
metals to improve the sensitivity, selectivity, and reaction recovery time of gas-sensing materials [16,17].

Based on the density functional theory (DFT) study, B, N-modified SnS2 is proposed as a promising sensor material for gas-sensing application in greenhouses, which can evaluate the change in concentration of NH3, Cl2, and C2H2 gases [18]. First, the most stable structure and the best modification performance of B, N-modified SnS2 was built and optimized [19]. Then, the most stable structure was chosen to analyze its adsorption mechanism to NH3, Cl2, and C2H2. By analyzing the structural optimization, adsorption energy, density of state (DOS), and charge transfer of gas molecules adsorption on B, N-modified SnS2, it is found that the modified SnS2 sensor shows high sensitivity to NH3, Cl2, and C2H2 [20,21]. This study provides a alternative approach for preparing SnS2-based gas sensors for the online monitoring of greenhouse gases [22–24].

2. Computational Details

All calculations were carried out based on DFT [23,25,26]. The SnS2 crystal plane is modeled with a 4 × 4 × 1 supercell [27–30]. To prevent the interaction from repeating planes along the z-axis direction, a vacuum layer of 25 Å was set between the planes [31,32]. The electron exchange and correlation energy were treated with the generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) basis [30]. A double numerical plus polarization (DNP) basis set was used [27]. The ionic convergence criterion for the total energy and maximum force were set as 1 × 10−5 Ha, and 2 × 10−3 Ha/Å, respectively [33,34], and the electronic self-consistent field tolerance was 1 × 10−6 Ha [30]. The Brillouin zone was sampled with a 5×5×1 Monkhorst-Pack mesh of k-points [33]. All calculations are performed under 0 K; the adsorption performance under room temperature is directly related to the results under 0 K.

The adsorption energy (Eads) of the molecule adsorbed on the SnS2 surface was calculated by Eads = E_slab/gas − E_slab − E_gas. E_slab/gas is the total energy of the adsorption system; E_slab and E_gas are the energy of the SnS2 surface and gas molecules of greenhouse gases, respectively [34]. A negative value of Eads means the adsorption process is exothermic and happens spontaneously [35]. The electron density distribution was calculated by Mulliken population analysis [36]. The charge transfer Q in the adsorption process was obtained by Q = Q_ads − Q_iso. Q_iso and Q_ads are the total charges of isolated gas and adsorbed gas molecules, respectively [37]. Q > 0 means electrons transfer from the gas molecules to the surface of SnS2. According to frontier molecular orbital theory, the gap energy represents the difference between the highest occupied orbital (HOMO) and the lowest occupied orbital (LUMO) [38]. The energy gap between HOMO and LUMO was defined by E_g = |E_HOMO − E_LUMO|1. The smaller the energy gap is, the more efficiently the reaction is excited.

3. Results and Discussion

3.1. Geometry Optimization

To obtain the adsorption characteristics of B-SnS2 and N-SnS2 to the greenhouse gases, the structures of the gas molecules and SnS2 surface were initially optimized. The structures of NH3, Cl2, and C2H2 gas molecules are established as shown in Figure 1a–c. The bond length of Sn-S in SnS2 is 2.611 Å. C2H2 gas molecule is a two-dimensional planar structure with only 1.211 Å C-C bond length and 1.071 Å C-H bond length. NH3 gas molecule is a regular tetrahedral structure: all of the N-H bond lengths are 1.023 Å, and the bond angles are 105.350°. Cl2 has a bond length of 2.024 Å. The two most stable modification structures of B and N modification on the SnS2 surface are obtained, respectively, as shown in Figure 1e,f. Based on the Mulliken population, B and N atoms as electron acceptors, 0.176 e electrons and 0.65 e electrons are obtained from SnS2. This redistribution of charge leads to a change in the system’s conductivity. It can be seen that the modification distance is 1.843 Å and 1.527 Å, respectively. From the bonding distance and charge transfer, both B
and N atoms have built a stable structure on the SnS$_2$ surface, which provides a foundation for further gas adsorption.

As shown in Figure 2, the total density of states (TDOS) and partial density of states (PDOS) are analyzed to further analyze the modification mechanism of the B and N atoms on SnS$_2$. Both B and N atom modifications make the TDOS move to the left. Therefore, after the modification of SnS$_2$ by B and N, the electrons in the conduction band are reduced, resulting in a decrease in the conductivity of SnS$_2$. According to the PDOS, the peaks of S-3$p$ and B-2$p$ overlap range from $-6$ eV to $-4$ eV, and at the 1 eV for the B-SnS$_2$ system. On the other hand, the peaks of S-3$p$ and N-2$p$ hybridize around $-5$ eV, $-4$ eV, $-2.5$ eV, 0 eV, and 2 eV. In general, the conductivity of the modified SnS$_2$ systems decreases due to the strong electronegativity of the modified atoms.

![Figure 1](image1.png)

**Figure 1.** The optimized structures: (a) NH$_3$, (b) Cl$_2$, (c) C$_2$H$_2$, (d) SnS$_2$, (e) B-SnS$_2$ surface, (f) N-SnS$_2$ surface. The distance is Å.

![Figure 2](image2.png)

**Figure 2.** (a1) TDOS of SnS$_2$ and B-SnS$_2$, (b1) TDOS of SnS$_2$ and N-SnS$_2$, (a2) PDOS of B-SnS$_2$, (b2) PDOS of N-SnS$_2$. 
As shown in Figure 3, after B and N modification on SnS2, HOMO is mainly distributed on B and N, indicating that B and N atoms provide electrons as electron donors and are active sites that can provide adsorption sites for NH3, Cl2, and C2H2 gases. Moreover, the energy gap increases significantly after modification as listed in Table 1, making the system’s conductivity significantly decrease; therefore, the measurement system’s conductivity change is more pronounced. The results obtained by the frontier molecular orbital theory are consistent with those obtained by the density of state analysis.

![Figure 3. HOMO and LUMO of (a) B-SnS2 and (b) N-SnS2.](image)

| Configuration  | Structure   | E_{HOMO} (eV) | E_{LUMO} (eV) | E_g (eV) |
|---------------|-------------|---------------|---------------|---------|
| B-SnS2        | Figure 3a   | -0.209        | -0.190        | 0.019   |
| N-SnS2        | Figure 3b   | -0.221        | -0.196        | 0.025   |

### 3.2. NH3, Cl2, and C2H2 Adsorption on B-SnS2 and N-SnS2 Surfaces

To study the adsorption properties of the three greenhouse gases on B-SnS2 and N-SnS2, NH3, Cl2, and C2H2 gases were made to approach the B-SnS2 and N-SnS2 surfaces from different positions to obtain the most stable adsorption structures. Figure 4 shows the most stable adsorption structures after gas molecules adsorption on B-SnS2.

![Figure 4. Gas adsorption on B-SnS2. (a) B-SnS2/NH3, (b) B-SnS2/Cl2, (c) B-SnS2/C2H2. The distance is Å.](image)

#### 3.2.1. Gas Adsorption on B-SnS2 Surface

Figure 4 and Table 2 show the optimal adsorption structure of NH3, Cl2, and C2H2 gas molecules on B-SnS2. Since the B atom is in a prominent position on the SnS2 surface, it provides a better attachment point for gas adsorption, making the adsorption of SnS2 more stable. The H and N atoms in the NH3 molecule were used to approach the surface of SnS2. The results showed that the H atom approaching the B atom method acts as the most stable structure with the largest adsorption energy (−1.735 eV). When the N atom is closed to the B atom, the adsorption energy is only −0.712 eV. The greater the absolute value of the adsorption energy, the more intense the reaction is. In addition, the negative adsorption energy means that the reaction is exothermic and can be carried out spontaneously. From the microscopic point of the adsorption structure, the bending stress also causes the surface deformation of B-SnS2 to different degrees. The adsorption distance of B-SnS2 to NH3 gas is 2.055 Å. The small adsorption distance indicates that the reaction may be strong...
chemisorption. After gas adsorption, SnS$_2$ has slight deformation, and the Sn-S bond is slightly elongated. After B-SnS$_2$ adsorbs NH$_3$ gas, 0.254 e electrons transfer from the H$_2$S gas to B-SnS$_2$, mainly provided by the H atom. After the Cl$_2$ adsorption on B-SnS$_2$, the adsorption energy is $-2.204$ eV, the charge transfer is $-0.422$ e, and the adsorption distance is 1.776 Å. The reaction is also chemical adsorption due to the large adsorption energy and shorter adsorption distance. Upon C$_2$H$_2$ adsorption on B-SnS$_2$, the adsorption distance is 2.531 Å, the adsorption energy is $-0.272$ eV, and the charge transfer is 0.172 e. It can be deduced that the C$_2$H$_2$ adsorption on B-SnS$_2$ belongs to physical adsorption.

Table 2. Adsorption parameters of gas molecules on B-SnS$_2$.

| System            | Structure   | $d$ (Å) | $E_{\text{ads}}$ (eV) | $Q_T$ (e) |
|-------------------|-------------|---------|------------------------|-----------|
| B-SnS$_2$/NH$_3$  | Figure 4a   | 2.055   | -1.735                 | 0.254     |
| B-SnS$_2$/Cl$_2$  | Figure 4b   | 1.776   | -2.024                 | -0.422    |
| B-SnS$_2$/C$_2$H$_2$ | Figure 4c | 2.531   | -0.272                 | 0.172     |

Figure 5 shows the DOS analysis diagram of B-SnS$_2$ after adsorption of NH$_3$, Cl$_2$, and C$_2$H$_2$; the TDOS after gas adsorption moves to the right, where the dotted line represents the Fermi energy level. From Figure 5(a1,a2), it can be figured out that the TDOS has a distinct increase above the Fermi level after NH$_3$ adsorption. It facilitates the transition of electrons from the valence band to the conduction band, resulting in an overall increase in conductivity. After NH$_3$ adsorption, the TDOS increases range from $-5$ eV to $-2.5$ eV, $-10$ eV to $-12.5$ eV, and 2.5 eV to 3 eV, respectively, which are caused by the hybridization of H-1$s$ and B-2$p$ orbitals. The strong orbital hybridization and the considerable TDOS increase indicate that this reaction is chemisorption. Additionally, the adsorption structure is very stable. When the Cl$_2$ molecule is adsorbed, the TDOS of B-SnS$_2$/Cl$_2$ shifts to the right as a whole, and the TDOS will increase at the energy level range of 0 eV, whereas the TDOS will decrease at the energy level range of $-15$ eV to $-12$ eV and $-5$ eV to $-2$ eV. The conductivity of the surface system enhances as the DOS at the Fermi level increases. The hybridization of the B-2$p$ orbital and Cl-3$p$ orbital shows that the reaction is very violent. According to the analysis of the DOS diagram shown in Figure 5(c1,c2), the distribution of TDOS nearly does not change before and after C$_2$H$_2$ adsorption.

![Figure 5](https://example.com/figure5.png)

Figure 5. (a1) TDOS of B-SnS$_2$ and B-SnS$_2$/NH$_3$. (b1) TDOS of B-SnS$_2$ and B-SnS$_2$/Cl$_2$. (c1) TDOS of B-SnS$_2$ and B-SnS$_2$/C$_2$H$_2$. (a2) PDOS of B-SnS$_2$/NH$_3$. (b2) PDOS of B-SnS$_2$/Cl$_2$. (c2) PDOS of B-SnS$_2$/C$_2$H$_2$. 
3.2.2. Gas Adsorption on N-SnS₂ Surface

Figure 6 shows the most stable structures of gas molecules on N-SnS₂. For NH₃ adsorption in Figure 6a, the structure of NH₃ keeps intact in the adsorption process. The most stable structure for NH₃ adsorption is obtained by the H atom of NH₃ closing the N atom of N-SnS₂, and the adsorption distance is 2.162 Å. The large adsorption distance indicates that the adsorption is physical adsorption. For Cl₂ adsorption in Figure 6b, Cl atoms approach the surface of N with a single Cl atom. The adsorption distance reaches 2.915 Å. In addition, the chemical bond in Cl₂ keeps intact in the adsorption process, only a slight elongation occurs in the Cl-Cl bond length, indicating that the adsorption is also weak physical adsorption. The adsorption structure of C₂H₂ is shown in Figure 6c. Its adsorption characteristics are similar to NH₃, and the adsorption distance is 2.361 Å. The structure of C₂H₂ has not been damaged during the adsorption process.

![Figure 6. Gas adsorption on N-SnS₂. (a) N-SnS₂/NH₃, (b) N-SnS₂/Cl₂, (c) N-SnS₂/C₂H₂. The distance is Å.](image)

The adsorption parameters of gases adsorbed N-SnS₂ systems are listed in Table 3, including adsorption distance, adsorption energy, and charge transfer. It can be seen from the table that the adsorption energy of NH₃ is −0.408 eV, and negative adsorption energy means that the reaction is exothermic and spontaneous. The charge transfer is 0.147 e, indicating a 0.147 e electron transfer from NH₃ to N-SnS₂. The small adsorption energy, long adsorption distance, and charge transfer confirm that the adsorption is physical adsorption. The adsorption energy of Cl₂ is −0.245 eV, which is the lowest among the three gas adsorption, and its charge transfer is −0.136 e. The adsorption energy of C₂H₂ is −0.272 eV, which is the most moderate among the three gases. In total, 0.197 e electrons have been transferred to C₂H₂ from N-SnS₂.

**Table 3.** Adsorption parameters of gas molecules on N-SnS₂.

| System          | Structure | d (Å) | \(E_{\text{ads}}\) (eV) | \(Q_T\) (e) |
|-----------------|-----------|-------|--------------------------|-------------|
| N-SnS₂/NH₃      | Figure 6a | 2.162 | −0.408                   | 0.147       |
| N-SnS₂/Cl₂      | Figure 6b | 2.915 | −0.245                   | −0.136      |
| N-SnS₂/C₂H₂     | Figure 6c | 2.361 | −0.272                   | −0.197      |

By comparing the adsorption of these three gases on B-SnS₂ and N-SnS₂, NH₃ and C₂H₂ always give electrons to the substrate, whereas Cl₂ always gains electrons. In addition, B-SnS₂ has larger adsorption energy, larger charge transfer amount, and a shorter adsorption distance for the Cl₂ adsorption system, indicating that the B-SnS₂ monolayer has the most robust adsorption performance for Cl₂ gas molecules. Based on the above analysis, it can be concluded that the modification of B enhances the adsorption activity of NH₃, Cl₂, and C₂H₂ to SnS₂. The adsorption capacity of B-SnS₂ to these gases is Cl₂ > NH₃ > C₂H₂.

As shown in Figure 7, TDOS and PDOS of all adsorbed gas systems were analyzed to further study the adsorption mechanism of the N-SnS₂ system to the gas molecules, where dotted lines represent Fermi energy levels. TDOS and PDOS of N-SnS₂ adsorption by NH₃, Cl₂, and C₂H₂ are shown in Figure 7(a1–c1) and Figure 7(a2–c2), respectively. For NH₃ adsorption, the TDOS of the adsorption system increases a little near the Fermi level. It indicates that the conductivity of the adsorption system increases slightly. The interaction between N-2p and H-1s is fragile. After Cl₂ adsorption, the atomic orbitals are strongly hybridized between the peaks of Cl-3p and N-2p. The TDOS of C₂H₂ nearly does
not change after C\textsubscript{2}H\textsubscript{2} adsorption on N-SnS\textsubscript{2}, and the corresponding interatomic orbital hybridization is also faint. Only the C-2\textit{p} and H-1\textit{s} peaks of the adsorption system overlap with the N atomic orbitals between −5.0 eV and −10.0 eV.

3.3. Analysis of Gas-Sensing Response

The behavior of electrons in the adsorption process was analyzed by frontier molecular orbital theory. The HOMO and LUMO were obtained after NH\textsubscript{3}, Cl\textsubscript{2}, and C\textsubscript{2}H\textsubscript{2} gas adsorption. It helps to explore gas sensors with selectivity and sensitivity. The HOMO and LUMO distributions before and after gas adsorption on B-SnS\textsubscript{2} are shown in Figure 8, and the energy gap values are shown in Table 4. The adsorption charge transfer of Cl\textsubscript{2} and NH\textsubscript{3} molecules is significant. The HOMO and LUMO distributions are improved by gas adsorption, part of HOMO and LUMO transfer to Cl\textsubscript{2} and NH\textsubscript{3} molecules. The specific charge numbers corresponding to the analysis of the three gases are 0.254 e, −0.422 e, and 0.172 e, respectively. The charge transfer amount during the analysis of the adsorption process mainly comes from modified B atoms. Overall, the energy gap upon Cl\textsubscript{2} and NH\textsubscript{3} adsorption on the surface of B-SnS\textsubscript{2} is bigger than that of C\textsubscript{2}H\textsubscript{2}. After adsorption, the energy gap value changes from 0.019 eV (B-SnS\textsubscript{2}) to 0.024 eV (B-SnS\textsubscript{2}/NH\textsubscript{3}), 0.014 eV (B-SnS\textsubscript{2}/Cl\textsubscript{2}), and 0.019 eV (B-SnS\textsubscript{2}/C\textsubscript{2}H\textsubscript{2}), respectively. A smaller energy gap indicates that the system’s conductivity improves, which is consistent with the previous DOS analysis.

Figure 8. HOMO and LUMO of gas-adsorbed B-SnS\textsubscript{2} systems: (a) B-SnS\textsubscript{2}/NH\textsubscript{3}, (b) B-SnS\textsubscript{2}/Cl\textsubscript{2}, (c) B-SnS\textsubscript{2}/C\textsubscript{2}H\textsubscript{2}.
Table 4. Energy of HOMO, LUMO, and energy gap of B-SnS$_2$ and adsorption systems.

| Configuration     | Structure | $E_{\text{HOMO}}$ (eV) | $E_{\text{LUMO}}$ (eV) | $E_g$ (eV) |
|-------------------|-----------|------------------------|------------------------|------------|
| B-SnS$_2$/NH$_3$  | Figure 8a | −0.203                 | −0.179                 | 0.024      |
| B-SnS$_2$/Cl$_2$  | Figure 8b | −0.211                 | −0.197                 | 0.014      |
| B-SnS$_2$/C$_2$H$_2$ | Figure 8c | −0.209                 | −0.190                 | 0.019      |

The HOMO and LUMO distributions before and after gas adsorption on N-SnS$_2$ are shown in Figure 9, and the energy gap values are shown in Table 5. HOMO is mainly distributed on N before N-SnS$_2$ adsorbs gas, indicating that the N atom provides electrons as electron donors and is also the active site that provides adsorption sites for NH$_3$, Cl$_2$, and C$_2$H$_2$ gas. After adsorbing NH$_3$, Cl$_2$, and C$_2$H$_2$ gases, the HOMO becomes more concentrated on N, and the LUMO is nearly not located on gas molecules. From the HOMO and LUMO distribution of NH$_3$ molecule adsorption, the $E_g$ of N-SnS$_2$/NH$_3$ decreases to 0.025 eV. In addition, HOMO electrons are mainly located at H and N atoms, whereas LUMO electrons do not change significantly, which is consistent with the result obtained from TDOS and PDOS analysis. In contrast, the energy gap of N-SnS$_2$/Cl$_2$ is reduced to 0.023 eV, because HOMO electrons are mainly concentrated around N atoms, indicating that the adsorption of Cl$_2$ molecules dramatically improves the conductivity and has better reactivity on N-SnS$_2$ surfaces. In the C$_2$H$_2$ system, LUMO mainly concentrates around N atoms with long N-H bonds, reaching −0.196 eV. The increase in LUMO also reduces the energy gap of the system to 0.026 eV, resulting in a decrease in the conductivity of the system.

Figure 9. HOMO and LUMO of gas-adsorbed N-SnS$_2$ systems: (a) N-SnS$_2$/NH$_3$, (b) N-SnS$_2$/Cl$_2$, (c) N-SnS$_2$/C$_2$H$_2$.

Table 5. Energy of HOMO, LUMO, and energy gap of N-SnS$_2$ and adsorption systems.

| Configuration     | Structure | $E_{\text{HOMO}}$ (eV) | $E_{\text{LUMO}}$ (eV) | $E_g$ (eV) |
|-------------------|-----------|------------------------|------------------------|------------|
| N-SnS$_2$/NH$_3$  | Figure 9a | −0.219                 | −0.196                 | 0.023      |
| N-SnS$_2$/Cl$_2$  | Figure 9b | −0.220                 | −0.195                 | 0.025      |
| N-SnS$_2$/C$_2$H$_2$ | Figure 9c | −0.222                 | −0.196                 | 0.026      |

4. Conclusions

The adsorption of NH$_3$, Cl$_2$, and C$_2$H$_2$ molecules on B-SnS$_2$ and N-SnS$_2$ surfaces has been studied based on DFT calculation. The adsorption structure, charge transfer, DOS, and molecular orbital were analyzed to study the influence of B and N modification on the gas sensitivity of SnS$_2$ monolayer to the gas molecules. Pristine SnS$_2$ has low adsorption energy and a long adsorption distance for NH$_3$, Cl$_2$, and C$_2$H$_2$ gas molecules. Compared with the pristine SnS$_2$, the adsorption capacity of the three gases on B-SnS$_2$ and N-SnS$_2$
is improved. The adsorption capacity of B-SnS$_2$ to these gases is Cl$_2$ > NH$_3$ > C$_2$H$_2$. The adsorption capacity of N-SnS$_2$ is NH$_3$ > C$_2$H$_2$ > Cl$_2$. TDOS and PDOS analysis results show that B-SnS$_2$ has the strongest interaction with Cl$_2$ and the weakest interaction with C$_2$H$_2$. Frontier molecular orbital analysis shows that the influence of gas molecules on the conductivity of the B-SnS$_2$ adsorption system is NH$_3$ > C$_2$H$_2$ > Cl$_2$. The influence order of gas molecules on the conductivity of the N-SnS$_2$ adsorption system is C$_2$H$_2$ > Cl$_2$ > NH$_3$. The results lay a theoretical foundation for developing B-SnS$_2$ and N-SnS$_2$ gas sensors for greenhouse gas detection.

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