Monitoring Gases Content in Modern Agriculture: A Density Functional Theory Study of the Adsorption Behavior and Sensing Properties of CO\(_2\) on MoS\(_2\) Doped GeSe Monolayer

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Abstract: The reasonable allocation and control of CO\(_2\) concentration in a greenhouse are very important for the optimal growth of crops. In this study, based on density functional theory (DFT), an MoS\(_2\)-GeSe monolayer was proposed to unravel the issues of the lower selectivity, poorer sensitivity and non-recyclability of traditional nanomaterial gas sensors. The incorporation of MoS\(_2\) units greatly enhanced the sensitivity of the pure GeSe monolayer to CO\(_2\) and the high binding energy also demonstrated the thermal stability of the doped structures. The ideal adsorption energy, charge transfer and recovery time ensured that the MoS\(_2\)-GeSe monolayer had a good adsorption and desorption ability. This paper aimed to solve the matter of recycling sensors within agriculture. This research could provide the theoretical basis for the establishment of a potentially new generation of gas sensors for the monitoring of crop growth.

Keywords: gas sensors; density functional theory; 2D materials; carbon dioxide

1. Introduction

In modern agriculture, greenhouses are often used to artificially change the growth environment of crops in order to cope with random and changeable weather conditions and ensure the diversity of seasonal agricultural products \cite{1-3}. The growth process of plants, carbon is an important organic matter, mainly in the form of CO\(_2\) \cite{4,5}. CO\(_2\) is a necessary material for plants, which plays a very important role in photosynthesis \cite{6-8}. It directly affects the normal growth of plants and the abundance of nutrients within plants. In addition, the concentration of CO\(_2\) can change the biological and abiotic conditions in soil to some extent \cite{9,10}. Increases in the emissions of potent greenhouse gases from soil under increasing atmospheric CO\(_2\) indirectly affect the growth of crops. Moreover, the demand for CO\(_2\) is different in different growth stages of crops. For example, in this study, demand for CO\(_2\) reached the maximum value of 1000–1200 ppm before sunrise and then decreased to about 100 ppm 2.5–3 h after sunrise, which was only about 30% of the atmospheric concentration. It did not begin to rise again until 2 h after sunrise and returned to the atmospheric level around 4 p.m. The concentration of carbon dioxide that is required for vegetables to grow is generally 1000–1500 ppm, so CO\(_2\) deficiency in a greenhouse is quite serious and has become an important factor that affects the yield of greenhouse vegetables. Therefore, the reasonable allocation and control of CO\(_2\) concentration in greenhouses are critical for the optimal growth of crops. Zhang et al. have conducted a lot of research on the study of density functional theory (DFT) \cite{11-16}. They studied the microscopic interactions between two-dimensional (2D) materials and gas molecules to explore the application of these materials as gas adsorbents and sensors, such as the use of an Au-doped graphene monolayer as a gas sensor \cite{13,16}. Other relevant work has proved that the simulation calculation is very consistent with experimental results. Based on DFT, we
theoretically designed a new type of CO\textsubscript{2} concentration detection sensor, which can be indirectly observed and used to control the growth of plants.

Compared to traditional gas sensors, the use of nanomaterial sensors for the detection of gas type and gas content has the advantages of small size, fast response, high sensitivity and low costs. Tao et al. explored the use of nanomaterial sensors, both in theory and experimentally [17–21]. Thanks to their large surface areas and adequate adsorption sites, 2D materials are increasingly being used as gas adsorbents and sensors and were studied by Gui et al. [22–25]. After graphene, GeSe monolayers have attracted a lot of interest as 2D materials with high optical responsiveness, high mobility and high flexibility. Zhou et al. also systematically explored the physical and chemical properties of a GeSe monolayer [26–28] and Dai et al. successfully prepared GeSe thin films [29]. Recently, several researchers have explored the use of GeSe monolayers as gas sensors or adsorbents. Liu et al. studied the gas adsorption characteristics of an intrinsic GeSe monolayer [30], but due to its weak adsorption ability, it could not provide enough of a theoretical basis for gas sensors. Tao et al. explored the adsorption characteristics of a modified GeSe monolayer for SF\textsubscript{6} decomposition gas by doping metal oxides [31–33]. However, despite being an important gas that is applied in various fields, CO\textsubscript{2} lacks theoretical exploration using GeSe-based monolayers. Li et al. found that the adsorption ability of Ce–CaO to CO\textsubscript{2} is too strong to be desorbed, which is not conducive to the recyclability of sensors [34–37]. The adsorption ability of Al–BN monolayers and graphene to CO\textsubscript{2} is also too small, which is the reason that they cannot obtain enough of a response [38,39]. Gui et al. proposed that metal oxide doping can effectively improve the gas selectivity and sensitivity of 2D materials [40,41], which offered the essential theoretical basis for our study.

Here, we innovatively propose the use of a MoS\textsubscript{2}–GeSe monolayer to detect CO\textsubscript{2} for the first time. Based on the first principle, parameters such as binding energy ($E_b$), adsorption energy ($E_{\text{ads}}$), charge transfer ($\Delta Q$), band gap ($E_g$), density of states (DOS), work functions (WFs), charge density difference (CDD), deformation charge density (DCD) and electron localization function (ELF) were analyzed. Doping with MoS\textsubscript{2} units caused the GeSe monolayer to have a higher sensitivity to CO\textsubscript{2} and an excellent thermal stability ($E_b = -5.994$ eV). For the better simulation of the practical applications of gas sensors, we analyzed the recovery time at different temperatures. Appropriate $E_{\text{ads}} (-0.955$ eV) and $\Delta Q (0.266$ e) values caused the MoS\textsubscript{2}–GeSe monolayer to maintain an excellent response and also produce great recovery characteristics (1.25 s in 398 K). This could provide solid theoretical support for the application of resistive chemical sensors in agriculture.

2. Methods

All calculations were performed using the DMOL\textsuperscript{3} and CASTEP frameworks [42,43]. The generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) exchange correlation function were selected for analysis [44]. The energy convergence accuracy, maximum force and maximum displacement were set as $1 \times 10^{-5}$ Ha, $2 \times 10^{-3}$ Ha/Å and $5 \times 10^{-3}$ Ha/Å, respectively. Considering the weak interaction between atoms in calculations, such as the van der Waals force, Grimme’s DFT-D was applied [45–48]. Double numerical polarization (DNP) was also selected at the basic setting of 3.5.

A $4 \times 4 \times 1$ GeSe monolayer supercell was constructed and optimized using the highest precision setting in the material studio software. The k-point samples of the Monkhorst–Pack grid were sampled at $6 \times 6 \times 1$ for geometry optimization and $10 \times 10 \times 1$ for electronic optimization. The size of the vacuum space between two adjacent sheets was set at the value of 15 Å in order to avoid interactions between periodic images. A self-consistent loop energy of $10^{-6}$ Ha, a global orbital cut-off radius of 5.0 Å and a smearing of 0.005 Ha were applied. In order to study the role of MoS\textsubscript{2} doping in the adsorption of CO\textsubscript{2} to the GeSe monolayer, we compared the most stable configurations of CO\textsubscript{2} that were adsorbed to the MoS\textsubscript{2}–GeSe monolayer. Our strategy was to calculate all typical adsorption structures and then the maximum adsorption energy would correspond to the most stable adsorption configuration.
$E_b$ was determined using Equation (1), as follows:

$$E_b = E_{\text{MoS}_2\text{-GeSe}} - E_{\text{GeSe}} - E_{\text{MoS}_2}$$  \hspace{1cm} (1)

where $E_{\text{MoS}_2\text{-GeSe}}$, $E_{\text{GeSe}}$ and $E_{\text{MoS}_2}$ represent the total energies of MoS$_2$–GeSe, pure GeSe and MoS$_2$ units, respectively.

$E_{\text{ads}}$ was calculated using Equation (2), as follows:

$$E_{\text{ads}} = E_{\text{CO}_2/\text{MoS}_2\text{-GeSe}} - E_{\text{CO}_2} - E_{\text{MoS}_2\text{-GeSe}}$$  \hspace{1cm} (2)

where $E_{\text{CO}_2/\text{MoS}_2\text{-GeSe}}$, $E_{\text{CO}_2}$ and $E_{\text{MoS}_2\text{-GeSe}}$ represent the energy of the total systems, CO$_2$ and the separated systems, respectively.

The charge amount was obtained using the Milliken charge analysis and $\Delta Q$ was determined using Equation (3), as follows:

$$\Delta Q = Q_a - Q_b$$  \hspace{1cm} (3)

where $Q_a$ and $Q_b$ represent the total charge of the gas molecules after and before adsorption, respectively.

3. Results

As shown in Figure 1d, CO$_2$ is a common compound in air that is composed of two oxygen atoms and a carbon atom, which are attached by a polar covalent bond. In Figure 1a,e, the ball–stick model structure of the pure GeSe monolayer is shown. GeSe monolayer are serrated black crystals that are similar to black phosphorus and belong to the orthogonal crystal system. After structural optimization, the Ge–Se bond lengths of the most stable GeSe monolayers were maintained at 2.641 and 2.544 Å. As shown in Figure 1b,f, the MoS$_2$ units were stably adsorbed to the GeSe monolayer surface and the $E_b$ value reached up to $-5.994$ eV, which indicated that a stable doping structure was formed with great thermal stability. In addition, the introduction of MoS$_2$ units caused the Ge atoms in the GeSe monolayer to shift upward, which was produced by the strong interaction between the MoS$_2$ units and the GeSe monolayer. As shown in Figure 1c,g, a stable structure with the maximum $E_{\text{ads}}$ value was finally selected after the calculation of eight different sites. For the metal oxide materials, we found the four intrinsic structures of ZnO, SnO$_2$, TiO$_2$ and WO$_3$ through a literature review and compared and explored the gas adsorption characteristics of CO$_2$ to these common metal oxides. The specific parameters are shown in Table 1. It was obvious that the $E_{\text{ads}}$ values of several metal oxides were much lower than those of the MoS$_2$–GeSe monolayer ($-0.955$ eV) using DFT calculations, which indicated that the MoS$_2$–GeSe monolayer had excellent response characteristics for CO$_2$ detection. For pure ZnO, WO$_3$ had some positive $E_{\text{ads}}$ values, which indicated that the reaction could not be carried out spontaneously nor could that material be used as a sensor.

![Figure 1](image-url). Geometric structures of the GeSe monolayer (a,e), the MoS$_2$–GeSe monolayer (b,f), the CO$_2$/MoS$_2$–GeSe monolayer (c,g) and CO$_2$ (d). The red circle is MoS$_2$ unit.
Table 1. The $E_{ads}$ values of different materials.

| 2D Materials | Gas  | $E_{ads}$ (eV) | Ref.  |
|--------------|------|--------------|------|
| ZnO          | CO$_2$ | 0.01         | 49   |
| ZnO          | CO$_2$ | 0.44         | 50   |
| SnO$_2$      | CO$_2$ | -0.663       | 51   |
| TiO$_2$      | CO$_2$ | -0.17        | 52   |
| ZrO$_2$      | CO$_2$ | -0.05        | 52   |
| WO$_3$       | CO$_2$ | 0.22         | 53   |

As shown in Figure 2a, the overall TDOS of the MoS$_2$–GeSe monolayer shifted to the right after doping with MoS$_2$ units, especially near the Fermi level, which indicated that the conductivity of the GeSe monolayer decreased. In addition, a new peak appeared at $-6$ eV, which lays the foundation for the gas adsorption reaction. After the CO$_2$ adsorption by the MoS$_2$–GeSe monolayer, the peak amplitudes at $-8.5$ eV, $-4$ eV, $-3$ eV and $1.7$ eV in the TDOS of the system increased slightly, which depended on the small regional state coating. This reflected the direct weak interactions between the two-dimensional materials and gases. We performed a PDOS analysis of the MoS$_2$–GeSe monolayer decomposition (Figure 2b). Obviously, the adsorbed CO$_2$ could not redistribute the surface charge of the MoS$_2$–GeSe monolayer or the electrical conductivity of the system, which revealed the corresponding response mechanisms of the gas sensor. As shown in Figure 2d, all elements showed high levels of hybridization and the orbitals were distributed between $-10$ and $2$ eV, where Ge–p, Se–p, O–p and C–p orbitals contributed greatly to the charge recombination. In short, this indicated that there was an interaction between CO$_2$, the MoS$_2$ units and the GeSe monolayer; however, it was generally a weak interaction, which conformed to the application prospects of the MoS$_2$–GeSe monolayer as a gas sensor.

Figure 2. The TDOS and PDOS analyses of the CO$_2$/MoS$_2$–GeSe monolayer. The Fermi level is set at zero. (a) TDOS of CO$_2$/MoS$_2$–GeSe monolayer. (b) PDOS of CO$_2$/MoS$_2$–GeSe monolayer. (c) PDOS of two CO$_2$. (d) PDOS of CO$_2$/MoS$_2$–GeSe monolayer with atoms.
In Figure 3a,d, the gain and loss of electron density are indicated by the blue and red regions, respectively. From the DCD distribution and ΔQ values, the gas molecules contributed 0.266 e to the material surface as electron donors and the electron density changed significantly between the different distribution regions. The electron density of the O atoms in CO₂ increased greatly, while the region around the C atom lost electrons. The analysis indicated that the C atom of the CO₂ molecule provided electrons not only to the two O atoms, but also to the O atom in the doped MoS₂ units. It was evident from this transfer that the adsorption reaction was both exothermic and self-generated, which guaranteed stable and efficient adsorption effects. Figure 3b,e represents the redistribution of the charge density of CDD after adsorption. The adsorbed CO₂ was charged positively overall and had purple areas around it, which indicated strong electron drainage. The separated charge build-up and exhaustion also confirmed the weak interaction between the gas and the adsorbent, with no new chemical bonds taking shape. As shown in Figure 3c,f, the ELF values were between −1 and 1, where −1 and 1 stand for very low electron density and completely limited electron density, respectively. It was found that stable O–Ge and Mo–Se bonds were formed between the MoS₂ units and GeSe monolayer, which further confirmed the stability of the doping structure. In addition, there was no significant regional fusion between the CO₂ and the MoS₂–GeSe monolayer, which suggested that the adsorption reaction was physical adsorption and showed the uniqueness of the MoS₂–GeSe monolayer as a gas sensor that allows for a faster response and recovery.

![Figure 3](image-url)

Figure 3. DCD (a), CDD (b) and ELF (c) on the MoS₂–GeSe monolayer and DCD (d), CDD (e) and ELF (f) on the CO₂/MoS₂–GeSe monolayer.

The energy of electrons in solids cannot be continuously valued, but some discontinuous energy bands can be valued. To conduct electricity, there must be free electrons or holes. The energy of free electrons is called the conduction band and the energy of free holes is called the valence band. When the bound electrons become free electrons or holes, they must obtain enough energy from the valence band for the conduction band. The minimum energy is $E_G$. In short, $E_G$ refers to the energy transfer between the lowest level of the conduction band and the highest level of the valence band [54–56]:

$$\sigma \propto A \times \exp \left( -\frac{\Delta E_G}{2kT} \right)$$

where $\sigma$ is the conductivity, $k$ is the Boltzmann constant ($1.38 \times 10^{-23}$ J/K), $A$ is a fixed parameter and $T$ is the temperature. The change in $E_G$ after an adsorption reaction can reflect the change in system conductivity and can further reflect the change in resistance value in practical applications. The $E_G$ value of the MoS₂–GeSe monolayer decreased after CO₂ adsorption, which indicated that the conductivity of the GeSe-based monolayer increased and the resistance value decreased. As shown in Figure 4a,c, the doping with
MoS$_2$ units reduced the conductivity of the GeSe monolayer and increased the $E_g$ value from 0.725 eV to 0.786 eV, which indicated that the MoS$_2$–GeSe monolayer maintained the excellent semiconductor characteristics and gas response characteristics of pure GeSe. However, the $E_g$ value of the pure GeSe monolayer after CO$_2$ adsorption changed very little (from 0.725 eV to 0.753 eV), which indicated that CO$_2$ had little effect on the electrical conductivity of the system (Figure 4b). In actual detection, it could be impossible to detect the resistance change of GeSe-based monolayer gas sensors using high precision instruments. The adsorption of CO$_2$ reduced the $E_g$ value of the MoS$_2$–GeSe monolayer to 0.667 eV, which indicated that the difficulty of electron transition from the top of the valence band to the bottom of the conduction band was reduced (Figure 4d). This helped us to observe the resistance change that was caused by the gas concentration more clearly. In contrast to the pure GeSe monolayer, the MoS$_2$–GeSe monolayer could be used as a gas sensor for CO$_2$ detection.

![Figure 4](image_url)

Figure 4. The $E_g$ values of the pure GeSe monolayer (a), the CO$_2$/GeSe monolayer (b), the MoS$_2$–GeSe monolayer (c) and the CO$_2$/MoS$_2$–GeSe monolayer (d); the change trend of $E_g$ (e).

WFs are a property of particular material surfaces, which indicate the minimum energy that is required for the surface to immediately move electrons to a point within a vacuum [57,58]. In gas interaction, this determines the aligned contact barrier between the gas molecules and specific surfaces. As shown in Figure 5a, the doping with MoS$_2$ units increased the WFs of the GeSe monolayer to 4.653 eV, which hindered the electronic affinity of the system. This phenomenon further proved that the electronic transition of the GeSe monolayer was more difficult and that the chemical properties of the system were more stable after doping with MoS$_2$ units. However, the introduction of CO$_2$ reduced the WFs of the system to 4.544 eV, which indicated that after the CO$_2$ was adsorbed, the difficulty of electron spillover from the vacuum reduced. This further guided the adsorption of the MoS$_2$–GeSe monolayer to CO$_2$. It also reflected the electrostatic attraction between the gas molecules and the adsorption system. It was this simultaneous attraction that led to the interaction between the CO$_2$ and the MoS$_2$–GeSe monolayer. In conclusion, gas adsorption could cause changes in WFs, which also proved the possibility of using a Kelvin probe microscope to detect WFs in the field of gas sensing. Zhang et al. also studied the process of gas adsorption using WFs [33,53,55–61]. Figure 5b presents the theoretical recovery time of CO$_2$ at different temperatures that were calculated. The recovery times of sensing materials are closely related to the exposed ambient temperature. The calculation formula that we used was as follows [62,63]:

$$\tau = v_0^{-1} \times \exp \left( -\frac{E_{ads}}{kT} \right)$$  

(5)
where \( k \) is the Boltzmann constant, \( \tau \) is the recovery time and \( v_0 \) is the attempt frequency (\( 10^{12} \text{s}^{-1} \)). The thermal environment offers more energy for the desorption process and fosters the further diffusion of molecules. At 298 K, the recovery time of \( \text{CO}_2 \) was 14400 s, which caused the sensor to become unrecyclable. At 398 K, the desorption time of \( \text{CO}_2 \) decreased to 1.25 s, which further illustrated the excellent performance of the \( \text{MoS}_2–\text{GeSe} \) monolayer as a gas sensor. We inferred that 398 K could be used as the optimum temperature for the sensor, which would make it possible to apply the \( \text{MoS}_2–\text{GeSe} \) monolayer in agriculture.

![Figure 5](image_url)

**Figure 5.** Change trend of WFs (a); recovery time at different temperatures (b).

### 4. Conclusions

In this work, the sensing properties of an \( \text{MoS}_2–\text{GeSe} \) monolayer for \( \text{CO}_2 \) detection were systematically studied based on DFT. Compared to the pure GeSe monolayer, the \( \text{MoS}_2–\text{GeSe} \) monolayer had a higher sensitivity to \( \text{CO}_2 \) and the variation in \( E_g \) increased by 661% (0.119/0.018 \times 100%). In practical applications, the \( \text{MoS}_2–\text{GeSe} \) monolayer would have a greater change in resistance values as a chemical resistance sensor than during testing. The main parameters are shown in Table 2. The large \( E_h \) value (−5.994 eV) indicated that the \( \text{MoS}_2 \) units and GeSe monolayer had excellent binding abilities. The thermal stability of the doped system was robust enough and the sensor could deal with changes in the ambient operating temperature. As can be seen from the DOS, the enriched orbital hybridization demonstrated the interaction between the \( \text{CO}_2 \) and the active atomic groups. The ideal \( E_{\text{ads}} \) (−0.955 eV), \( \Delta Q \) (0.266 e) and recovery time (1.25 s in 398 K) not only ensured the detection ability of the \( \text{MoS}_2–\text{GeSe} \) monolayer as a sensor, but also ensured its excellent recyclability. This is an advantage that most two-dimensional material gas sensors do not have. Based on this theoretical investigation, we will proceed to test flexible patch gas sensors for the monitoring of crop growth.

|                     | \( E_h \)  | \( E_{\text{ads}} \) | \( \Delta Q \) | WFs       | Recovery Time |
|---------------------|------------|----------------------|----------------|-----------|---------------|
| \( \text{MoS}_2–\text{GeSe} \) Monolayer | −5.994 eV  | /                    | /              | 4.653 eV  | 14,400 s (298 K) |
| \( \text{CO}_2/\text{MoS}_2–\text{GeSe} \) Monolayer | /          | −0.955 eV            | 0.266          | 4.544 eV  | 28.2 s (358 K)  |
|                     |            |                      |                |           | 1.25 s (398 K)  |

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References

1. Alvarado, K.A.; Mill, A.; Pearce, J.M.; Vocaet, A.; Denkenberger, D. Scaling of greenhouse crop production in low sunlight scenarios. *Sci. Total Environ.* 2020, 707, 136012. [CrossRef] [PubMed]

2. Rodriguez, F.; Berenguel, M.; Guzmán, J.L.; Ramírez-Arias, A. *Modeling and Control of Greenhouse Crop Growth*; Springer: Berlin/Heidelberg, Germany, 2015.

3. Timmermans, G.H.; Hemming, S.; Baeza, E.; Van Thoor, E.A.; Schenning, A.P.; Debije, M.G. Advanced optical materials for sunlight control in greenhouses. *Adv. Opt. Mater.* 2020, 8, 2000738. [CrossRef]

4. Körner, C. Plant CO₂ responses: An issue of definition, time and resource supply. *New Phytol.* 2006, 172, 393–411. [CrossRef] [PubMed]

5. Pritchard, S.G.; Rogers, H.H.; Prior, S.A.; Peterson, C.M. Elevated CO₂ and plant structure: A review. *Glob. Change Biol.* 1999, 5, 807–837. [CrossRef]

6. Gerhart, L.M.; Ward, J.K. Plant responses to low [CO₂] of the past. *New Phytol.* 2010, 188, 674–695. [CrossRef]

7. Leakey, A.D.; Ainsworth, E.A.; Bernacchi, C.J.; Rogers, A.; Long, S.P.; Ort, D.R. Elevated CO₂ effects on plant carbon, nitrogen, and water relations: Six important lessons from FACE. *J. Exp. Bot.* 2009, 60, 2859–2876. [CrossRef]

8. Morison, J.; Lawlor, D. Interactions between increasing CO₂ concentration and temperature on plant growth. *Plant Cell Environ.* 1999, 22, 659–682. [CrossRef]

9. Bazzaz, F.; McConaughay, K. Plant plant interactions in elevated CO₂ environments. *Aust. J. Bot.* 1992, 40, 547–563. [CrossRef]

10. Makino, A.; Mae, T. Photosynthesis and plant growth at elevated levels of CO₂. *Plant Cell Physiol.* 1999, 40, 999–1006. [CrossRef]

11. Cui, H.; Zhang, X.; Li, Y.; Chen, D.; Zhang, Y. First-principles insight into Ni-doped InN monolayer as a noxious gases scavenger. *Appl. Surf. Sci.* 2019, 494, 1267. [CrossRef]

12. Cui, H.; Zhang, X.; Zhang, G.; Tang, J. Pd-doped MoS₂ monolayer: A promising candidate for DGA in transformer oil based on DFT method. *Appl. Surf. Sci.* 2019, 470, 1035–1042. [CrossRef]

13. Cui, H.; Zheng, K.; Xie, Z.; Yu, J.; Chen, X. Tellurene Nanoflake-Based NO₂ Sensors with Superior Sensitivity and a Sub-Parts-per-Billion Detection Limit. *ACS Appl. Mater. Interfaces* 2020, 12, 47704–47713. [CrossRef] [PubMed]

14. Hao, C.; Guozi, Z.; Xiaozheng, Z.; Ju, Y. Rh-doped MoSe₂ as toxic gas scavenger: A first-principles study. *Nanoscale Adv.* 2018, 1, 772–780.

15. Heping, C.; Kai, Z.; Yingying, Z.; Huaiyu, Y.; Xianping, C. Superior Selectivity and Sensitivity of C₇N Sensor in Probing Toxic Gases NO₂ and SO₂. *IEEE Electron Device Lett.* 2017, 39, 284–287.

16. Zhang, X.; Yu, L.; Wu, X.; Hu, W. Experimental Sensing and Density Functional Theory Study of H₂S and SOF₂ Adsorption on Au-Modified Graphene. *Adv. Sci.* 2015, 2, 1500101. [CrossRef]

17. Gui, Y.; Sun, H.; Wei, H.; Duan, S.; Tang, C.; Zhang, X. Effect of nickel doping on adsorption of SF₆ decomposition products over MoS₂ surface. *JOM* 2019, 71, 3971–3979. [CrossRef]

18. Jiang, T.; He, Q.; Bi, M.; Chen, X.; Sun, H.; Tao, L. First-principles calculations of adsorption sensitivity of Au-doped MoS₂ gas sensor to main characteristic gases in oil. *J. Mater. Sci.* 2021, 56, 13673–13683. [CrossRef]

19. Peng, Z.; Tao, L.-Q.; Zheng, K.; Yu, J.; Wang, G.; Sun, H.; Zhu, C.; Zou, S.; Chen, X. Gas Sensor Based on Semihydrogenated and Semifluorinated h-BN for SF₆ Decomposition Components Detection. *IEEE Trans. Electron Devices* 2021, 68, 1878–1885. [CrossRef]

20. Sun, H.; Gui, Y.; Wei, H.; Long, Y.; Wang, Q.; Tang, C. DFT study of SF₆ decomposed products on Pd–TiO₂: Gas sensing mechanism study. *Adsortion* 2019, 25, 1643–1653. [CrossRef]

21. Xia, S.-Y.; Tao, L.-Q.; Jiang, T.; Sun, H.; Li, J. Rh-doped h-BN monolayer as a high sensitivity SF6 decomposed gases sensor: A DFT study. *Appl. Surf. Sci.* 2021, 536, 147965. [CrossRef]

22. Liu, Z.; Gui, Y.; Xu, L.; Chen, X. Adsorption and sensing performances of transition metal (Ag, Pd, Pt, Rh, and Ru) modified WSe₂ monolayer upon SF₆ decomposition gases (SOF₂ and SO₂F₂). *Appl. Surf. Sci.* 2022, 581, 152365. [CrossRef]

23. Liu, Z.; Gui, Y.; Xu, L.; Chen, X. Adsorption and gas-sensing properties of Aun (n = 1–3) cluster doped MoTe₂ for NH₃, NO₂, and SO₂ gas detection. *Surf. Interfaces* 2022, 30, 101883. [CrossRef]

24. Wang, X.; Gui, Y.; Ding, Z.; Xu, H.; Zeng, H.; Chen, X. Density functional theory study of Pd, Pt, and Au modified GeSe for adsorption and sensing of dissolved gases in transformer oil. *Surf. Interfaces* 2022, 31, 101994. [CrossRef]

25. Wang, X.; Gui, Y.; Sun, N.; Ding, Z.; Chen, X. A DFT calculation: Gas sensitivity of defect GeSe to air decomposition products (CO, NO, and NO₂). *IEEE Sens. J.* 2022, 19, 905.

26. Hu, Y.; Zhang, S.; Sun, S.; Xie, M.; Cai, B.; Zeng, H. GeSe monolayer semiconductor with tunable direct band gap and small carrier effective mass. *Appl. Phys. Lett.* 2015, 107, 122107. [CrossRef]

27. Li, Z.; Liu, X.; Wang, X.; Yang, Y.; Liu, S.-C.; Shi, W.; Li, Y.; Xing, X.; Xue, D.-J.; Hu, J.-S. Strain-engineering the in-plane electrical anisotropy of GeSe monolayers. *Phys. Chem. Chem. Phys.* 2020, 22, 914–918. [CrossRef]

28. Zhao, H.; Mao, Y.; Mao, X.; Shi, X.; Xu, C.; Wang, C.; Zhang, S.; Zhou, D. Band structure and photoelectric characterization of GeSe monolayers. *Adv. Funct. Mater.* 2018, 28, 1704855. [CrossRef]
60. Zhou, Q.; Zhang, G.; Tian, S.; Zhang, X. First-Principles Insight into Pd-Doped ZnO Monolayers as a Promising Scavenger for Dissolved Gas Analysis in Transformer Oil. *ACS Omega* 2020, 5, 17801–17807. [CrossRef]

61. Cui, H.; Yan, C.; Jia, P.; Cao, W. Adsorption and sensing behaviors of SF₆ decomposed species on Ni-doped C₃N monolayer: A first-principles study. *Appl. Surf. Sci.* 2020, 512, 145759. [CrossRef]

62. Cui, H.; Jia, P.; Peng, X.; Li, P. Adsorption and sensing of CO and C₂H₂ by S-defected SnS₂ monolayer for DGA in transformer oil: A DFT study. *Mater. Chem. Phys.* 2020, 249, 123006. [CrossRef]

63. Chen, D.; Zhang, X.; Tang, J.; Cui, Z.; Cui, H. Pristine and Cu decorated hexagonal InN monolayer, a promising candidate to detect and scavenge SF₆ decompositions based on first-principle study. *J. Hazard. Mater.* 2019, 363, 346–357. [CrossRef] [PubMed]