Adsorbed Behavior of Ni-Doped ZnO Monolayer upon SF$_6$ Decomposed Components and Effect of the Applied Electric Field

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1. INTRODUCTION

Over the last decade, many novel two-dimensional (2D) materials with physicochemical properties comparable to and even more superior than those of graphene are successfully isolated as potential candidates for applications in the fields of gas sensing, energy storage, and catalysis.

Recently, graphene-like zinc oxide (ZnO), belonging to the II–VI semiconducting materials, has attracted remarkable attention as a result of its large surface area and electronic motion, which especially motivate its application as a chemical sensor for gas detection. Combined with the theoretical prediction for the ZnO monolayer as a sensing material for H$_2$S detection, there are also experimental findings on ZnO nanosheets for NO$_2$ sensing. Furthermore, the single-layer ZnO is reported to be successfully synthesized on the Au(111) surface, which forebodes its potential for gas sensing purposes and application in many fields.

In the field of electrical engineering, SF$_6$ is widely applied in high-voltage devices as an insulation medium while the long-run, the inevitable insulation faults, such as partial discharge and partial overheat decompose SF$_6$ gas, leading to the formation of some stable chemicals when interacting with trace H$_2$O and O$_2$ in the devices. Reports indicate that under partial discharge, the main SF$_6$ decomposed components include SOF$_2$, and SO$_2$, while under partial overheating, the content of H$_2$S dramatically increases. It has been proved that the existence of these decompositions deteriorates the insulation performance of SF$_6$ and thus poses a great threat to the safe running of the insulation devices. Therefore, the sensing of these decomposed species is proposed to monitor the decomposition status of SF$_6$ and to reflect related insulation faults of the devices, which would be beneficial to take corresponding measures for equipment maintenance.

Certainly, the chemical sensing method with merits of rapid response, low cost, and good sensitivity could be engaged for such mission to detect these typical gases and has been regarded as one of the most workable approaches to this end.

Up to now, ZnO-based gas sensors, to the best of our knowledge, have not been exploited and investigated for detection of SF$_6$ decomposed components, and the desirable chemical reactivity of ZnO monolayer in gas interaction predicted in ref stimulates us to perform related theoretical calculations to explore its application for sensing SF$_6$ decompositions. Moreover, ref indicates that transition-metal (TM)-doped pristine ZnO monolayers show much stronger catalytic and sensing performances in gas interactions since the TM dopants can effectively promote the carrier mobility and charge-transferring property of the nanosup-

**ABSTRACT:** In this article, Ni-doped ZnO (Ni-ZnO) monolayer is proposed as a potential sensing material for detection of two SF$_6$ decomposed components (namely, SO$_2$ and SOF$_2$), based on the density functional theory (DFT) method, to monitor the operation status of SF$_6$ insulation devices in the power system. The Ni-doping effect on the physicochemical properties of the pure ZnO monolayer is first studied, with the binding energy ($E_b$) calculated as $-1.49$ eV. Then, the adsorption of a Ni-ZnO monolayer upon SO$_2$ and SOF$_2$ molecules shows that the Ni-ZnO monolayer exhibits strong chemisorption upon the two gas species, with the adsorption energy ($E_a$) obtained as $-2.38$ and $-2.19$ eV, respectively. The electronic properties of the Ni-ZnO monolayer upon gas adsorption are studied through the density-of-state (DOS) analysis, whereas the band structure (BS) and work function (WF) analysis provide the sensing mechanism of the Ni-ZnO monolayer. In addition, the charge-transfer behavior during adsorption in the applied electric fields is analyzed to expound the possibility of Ni-ZnO monolayer as a field-effect-transistor gas sensor. Our calculations can stimulate the study on adsorption and sensing behaviors of TM-ZnO monolayers for their applications in many fields.
ports. In this regard, the sensing response of TM-ZnO monolayers would be larger than that of the pure counterpart, suggesting its better suitability as a gas sensor. Given the desirable catalytic behavior of Ni atoms in gas adsorption, we propose the Ni-doped ZnO (Ni-ZnO) monolayer as a chemical gas sensor in this work, for detecting the main typical gases of SF₆ decompositions under partial discharge (SO₂ and SOF₂).

The Ni-doping effect on the geometric and electronic behaviors of the pure ZnO surface is first investigated, and the adsorption performance of the Ni-ZnO monolayer upon SO₂ and SOF₂ is simulated subsequently. Then, the sensing mechanism of the Ni-ZnO monolayer is put forward to elucidate its application as a gas sensor to monitor the partial discharge of SF₆ in high-voltage devices. Also, the charge-transfer behavior between the Ni-ZnO monolayer and gas molecules in the applied electric fields is analyzed to expound its possibility as a field-effect-transistor gas sensor. We hope that this work can stimulate further exploration of TM-ZnO monolayers as chemical sensors in many fields.

2. RESULTS AND DISCUSSION

3.1. Analysis of Ni-ZnO Monolayer. Using the established ZnO supercell, we first obtain its optimized geometric structure as shown in Figure 1a. The constant lattice of the ZnO monolayer is obtained as 3.30 Å in this work with the Zn−O bond length measured as 1.91 Å, in agreement with the theoretical work. To effectively find out the preferred Ni-doping site on the pristine ZnO monolayer, the frontier molecular orbital theory is applied, which can show the distributions of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) that have strong reactivity. With these results, the HOMO and LUMO of pristine ZnO are exhibited in Figure 1b,c, respectively. From these two figures, one can see that both HOMO and LUMO are mainly localized on the O atom, and there are some HOMOs on the Zn atoms, indicating the stronger chemical reactivity of O atoms when interacting with the surroundings compared with the Zn atoms. Besides, the energies of HOMO and LUMO of the ZnO monolayer are calculated to be −5.53 and −3.67 eV, respectively. This finding indicates the energy gap of 1.86 eV for the pristine ZnO system, which agrees with its semiconducting property well.

According to the frontier molecular orbital analysis, we could find that both Zn and O atoms are chemically reactive and are the possible sites for Ni-doping, as traced as T_O (at the top of the O atom) and T_Zn (at the top of the Zn atom) sites on the ZnO surface. Moreover, the binding energy ($E_b$) is calculated to evaluate the force between the Ni dopant and the ZnO surface as

$$E_b = E_{\text{Ni-ZnO}} - E_{\text{Ni}} - E_{\text{ZnO}}$$

where $E_{\text{Ni-ZnO}}$, $E_{\text{Ni}}$, and $E_{\text{ZnO}}$ represent the energies of the Ni-ZnO surface, isolated Ni atom, and pure ZnO surface, respectively.

After full optimization, it is found that the Ni dopant prefers to be trapped on the T_O site of the ZnO monolayer, which has a
lower $E_{	ext{ad}}$ indicating its stronger stability. The related configuration is depicted in Figure 2a,b. It is seen that on the $T_0$ site, the Ni dopant is trapped by the O atom and the surrounding Zn atoms, with the Ni–Zn bonds measured as 2.61 Å and the Ni–O bond measured as 1.84 Å. Besides, the ZnO monolayer experiences slight deformation around the Ni center due to the strong binding force between the Ni dopant and the ZnO surface, as supported by the large $E_b$ of 1.49 eV. These findings manifest the chemisorption of a Ni atom onto the pure ZnO monolayer.28 Based on the Hirshfeld analysis, the Ni dopant is negatively charged by 0.013e, implying the electron-accepting behavior of the Ni atom here, agreeing with the deformation charge density (DCD) in Figure 2c, wherein the Ni dopant is mainly embraced by electron accumulation.

The band structure (BS) and density of state (DOS) of the Ni-ZnO monolayer are plotted in Figure 2d–f to illustrate its electronic behavior. In the BS, it is seen that the band gap of the Ni-doped system is 1.100 eV, much smaller than that of 1.867 eV in the pure counterpart.29 This finding indicates that Ni-doping induces significant impurity states within the band gap of the pure ZnO system and thus narrows the band gap in the Ni-doped system. Moreover, the reduction of band gap in the Ni-ZnO monolayer suggests the enhancement of its electrical conductivity in comparison with the pure ZnO monolayer. From the total DOS, one can see that the Ni dopant contributes largely to the total DOS of the system, including the states around $-0.7$, $-0.2$, and 1.0–4.0 eV. Thus, there appear novel states in the Ni-ZnO system around the Fermi level that deform the electronic property of the pure ZnO system largely. However, the semiconducting property is not changed for the ZnO monolayer with Ni-doping according to the BS analysis. The desirable increase in the carrier mobility reflects the enhanced chemical reactivity of the Ni-ZnO monolayer upon the gas molecules in the interactions. In addition, the atomic DOS shows that there are strong orbital hybridizations between the Ni 3d orbital and the Zn 3d orbital at around $-6$ eV while between the Ni 3d orbital and the O 2p orbital at around $-4$ eV and the Fermi level, which illustrates the strong binding force of Ni–Zn and Ni–O bonds. This is in good agreement with the findings based on the geometric structure of $E_b$.

### 3.2. Adsorption of $\text{SO}_2$ and $\text{SOF}_2$

The adsorption behavior of Ni-ZnO monolayer upon $\text{SO}_2$ and $\text{SOF}_2$ is conducted to analyze its potential as a chemical gas sensor, in which the $\text{SO}_2$ and $\text{SOF}_2$ molecule are approaching to the Ni dopant with various configurations to investigate the interaction between such two gas molecules and the Ni atom. Also, the adsorption energy ($E_{\text{ad}}$) is calculated to evaluate the interaction strength between the Ni-ZnO monolayer and the gas molecules, as well as to identify the most stable configuration (MSC) for gas adsorption, as

$$E_{\text{ad}} = E_{\text{Ni–ZnO/gas}} - E_{\text{Ni–ZnO}} - E_{\text{gas}}$$

where $E_{\text{Ni–ZnO/gas}}$, $E_{\text{Ni–ZnO}}$, and $E_{\text{gas}}$ signify the energies of the gas-adsorbed, the pure Ni-ZnO monolayer, and the isolated gas molecule, respectively. For the following analysis, we only plot the MSC and related charge density difference (CDD) for gas adsorption to better understand the charge transfer and bonding mechanism in various systems, as described in Figure 3.

For $\text{SO}_2$ adsorption onto the Ni-ZnO surface, the MSC is portrayed in Figure 3a1,a2, in which the $\text{SO}_2$ molecule is vertical to the ZnO surface with the S atom trapped by the Ni dopant, forming a Ni–S bond measured as 1.98 Å. The structures of the Ni-ZnO monolayer and the $\text{SO}_2$ molecule experience slight deformations, indicating the geometric activation in adsorption. The Ni–S bond length is much shorter than the summed covalent radii of these two atoms (2.13 Å31), implying the strong binding force between Ni and S atoms. Besides, the $E_{\text{ad}}$ is calculated as $-2.38$ eV, much larger than that of $-1.52$ eV for $\text{SO}_2$ adsorption through the O-end position. Thus, this adsorption configuration could be identified as chemisorption between the Ni-ZnO monolayer and the $\text{SO}_2$ surface, which further confirms the strong interaction of the Zn–S bond. According to the Hirshfeld analysis, the Ni dopant is negatively charged by 0.090e, while the $\text{SO}_2$ molecule as a whole is negatively charged by 0.183e. That is, the Ni dopant releases 0.04e and the ZnO plane releases 0.143e to the $\text{SO}_2$ molecule, implying its strong electron-accepting property as verified in ref 31. Also, it could be inferred that the Ni dopant behaves as a medium bridging the charge transfer from the ZnO surface to the $\text{SO}_2$ molecule, which could be attributed to the strong electron mobility of the Ni dopant. From the CDD in Figure 3c, it is found that electron accumulation is mainly on the $\text{SO}_2$ molecule and the Ni–S bond, while the electron depletion is mainly on the Ni dopant. These results not only support the Hirshfeld analysis but also verify the strong electron hybridization on the Ni–S bond, which facilitates the formation of a chemical bond.
As for the Ni-ZnO/SOF$_2$ system, it is found that the MSC in Figure 3b1,b2 is similar to that of the Ni-ZnO/SO$_2$ system mentioned above, in which the SOF$_2$ molecule stands on the top of the Ni atom through the S-end position with the S atom trapped by the Ni dopant. The geometric deformations on the SOF$_2$ molecule and the Ni-ZnO surface could be identified after adsorption as well, and the shorter length of the newly formed Ni–S bond here (1.95 Å) seems to elucidate the stronger binding force of the Ni–S bond compared with that in the SO$_2$ system. On the other hand, the $E_{ad}$ in the SOF$_2$ system ($-2.19$ eV) is not as large as that for SO$_2$ adsorption on the Ni-ZnO surface. Interestingly, when the SOF$_2$ molecule approaches the Ni dopant through the O- or F-end position, the molecule undergoes remarkable displacement and remains to be the S-end position with similar $E_{ad}$ calculated. However, it could signify the chemisorption in the SOF$_2$ system. Based on the Hirshfeld method, the Ni dopant is negatively charged by 0.109e, while the SOF$_2$ molecule is negatively charged by 0.148e after adsorption. The smaller charge transfer in the SOF$_2$ system suggests the weaker electron-accepting behavior of the SOF$_2$ molecule than that of the SO$_2$ molecule. Meanwhile, the ZnO plane plays the dominant role in releasing electrons to the gas molecule, while the Ni dopant plays the role of a bridge enhancing the charge transfer, which is the same as that in the SO$_2$ system. Due to the electron redistribution, the Ni dopant is embraced by electron depletion and the SOF$_2$ molecule and the Ni–S bond are embraced by electron accumulation, as plotted in Figure 3b3, which supports the Hirshfeld analysis properly.

3.3. Electronic Properties. Figure 4 displays the DOS distribution of the Ni-ZnO monolayer upon SO$_2$ and SOF$_2$ adsorption to expound its electronic properties in gas interactions. One can see that after adsorption, the total DOS of the Ni-ZnO monolayer undergoes significant deformation. Similarly in the two systems, the state at the top of the valence band is weakened, whereas the state at the bottom of the conduction band is right-shifted. In this case, the band gap of the Ni-ZnO monolayer is supposed to be increased after interaction with the SO$_2$ or SOF$_2$ molecule, which is further analyzed in the next section. At the same time, the interactions also deform and activate the electronic behavior of the adsorbed gas molecules. Taking SO$_2$ molecule as an example, the state at 3.0 eV is left-shifted to the place at around 1.7 eV, the state at 7.3 eV splits into several small states localized at around 4.2 eV, and the states at
around −1.4 eV to the Fermi level are split and left-shifted to
several novel states ranging from −4.1 to −0.2 eV.

Furthermore, the Ni 3d orbital and the S 2p orbital in the
atomic DOS are effectively hybrid around the Fermi level and
1.8 eV for the SO2 system, and around the Fermi level and 2.1 eV
for the SOF2 system. These findings imply the strong orbital
interaction between the Ni dopant and the S atom that leads to
the formation of Ni−S bonds in the two systems. Also, the top of
the valence band is mainly localized on the Ni dopant, while the
bottom of the conduction band is mainly on the S atom, which
indicates the charge transfer from the Ni dopant to the sulfides
and thus confirms the results based on the Hirshfeld analysis.

3.4. Sensor Exploration. Given the deformation in the
electronic behavior of the Ni-ZnO monolayer upon gas
adsorption, its band gap and work function (WF) could also
be affected, which are regarded as the workable and important
parameters to realize the resistance-type and field-effect
transistor sensor for gas detection, respectively. Thus, we
perform the band structure (BS) and WF calculation and give a
detailed analysis in this section to explore the possibility of the
Ni-ZnO monolayer as a gas sensor.

As exhibited in Figure 5a,b, the band gaps for SO2 and SOF2
systems are obtained as 1.515 and 1.547 eV, respectively. In
other words, the band gap of the Ni-ZnO monolayer is increased
by 37.7% after SO2 adsorption and by 40.6% after SOF2
adsorption. According to eq 3, the increase of band gap
decreases with the increase of the electric field strength changes.

\[ \sigma = A \times e^{(-B/e^{2kT})} \] (3)

Thus, such an apparent increase in the band gap of the Ni-
ZnO monolayer would lead to a significant decrease in its
electrical conductivity, and the changed electrical conductivity in
the two systems is large enough for detection by the
 electrochemical devices. In this regard, the Ni-ZnO monolayer is
a promising sensing material for detection of SO2 and SOF2 with
desirable electrical responses.

In Figure 5c, where the WF values of the Ni-ZnO monolayer
before and after SO2 and SOF2 adsorption are displayed, it is
seen that the WF of the isolated Ni-ZnO monolayer is obtained as
4.68 eV, which is much smaller than that of 5.44 eV for the
pristine ZnO system. Thus, we can conclude that Ni-doping
significantly facilitates the carrier density and carrier mobility of
the ZnO surface, thereby reducing its electron affinity and
making it easier to dislodge an electron from the Ni-doped
surface. After adsorption of SO2 and SOF2, the WF values of the
Ni-ZnO monolayer is increased to 5.44 and 5.34 eV,
respectively. Such results suggest that the electron overflow from
the Ni-ZnO monolayer to the vacuum level will be
impeded after gas adsorption. At the same time, the changed WF
of the Ni-ZnO monolayer induced by SO2 and SOF2 adsorption
sheds light on the possibility of their detection by Kelvin probe
microscopy, which focuses on WF monitoring, or the
field-effect-transistor sensor, which can modulate the gate voltage and
thus amplify the sensing response.

3.5. Effect of the Electric Field. \( Q_f \) in gas adsorption plays a
major role in modulating the electrical conductivity of a
sensing material and determines the performance of the
field-effect-transistor sensor. To further study the sensing behavior of
the Ni-ZnO monolayer upon SO2 and SOF2 molecules, the effect of the applied electric field is investigated in this section. Figure 6a shows the schematic of the applied electric field, where the arrows represent the positive direction, while Figure 6b exhibits related \( Q_f \) in SO2 and SOF2 systems with the change of the
electric field strength.

From Figure 6, it could be found that the \( Q_f \) from the Ni-ZnO
monolayer to the gas molecules become increased with the
increase of the field strength along the negative direction. While
the \( Q_f \) from the SO2 or SOF2 molecule to the Ni-ZnO surface
decreases with the increase of the field strength along the
positive direction, the \( Q_f \) becomes positive, indicating the
converse charge transfer from the gaseous molecules to the Ni-
ZnO surface. In other words, the positive electric field drives the
electrons from the molecule to the Ni-ZnO monolayer when its
field strength is beyond a critical value. As the SO2 and SOF2
molecules attach 0.062 and 0.084e from the Ni-ZnO surface at 0.25 V/Å and release 0.036 and 0.011e, respectively, to the Ni-ZnO surface at 0.25 V/Å, it is predicted that the critical value to tune the charge-transferring path could be located at around 0.41 V/Å for the SO2 system and 0.47 eV for the SOF2 system. Moreover, the dependence of \( Q_f \) on the electric field direction may probably be responsible for the dipole moment of the molecule–monolayer system, which provides reliable evidence for the enhancement of sensing response by a field-effect-transistor gas sensor.
3. CONCLUSIONS

In this work, the DFT method is employed to investigate the potential of the Ni-ZnO monolayer as a novel sensing material for detecting two SF$_6$ decomposed components (SO$_2$ and SOF$_2$), for exploring a novel sensing material for monitoring the operation status of SF$_6$ insulation devices. The main conclusions are as follows:

i. The frontier molecular orbital theory indicates the strong interaction of the $T_{Zn}$ site with the impurities, on which the Ni dopant is captured with $E_b$ of $-1.49$ eV.

ii. The Ni-ZnO monolayer exhibits chemisorption upon SO$_2$ and SOF$_2$ adsorption, with $E_{ad}$ of $-2.38$ and $-2.19$ eV, respectively.

iii. The BS analysis sheds light on the potential of the Ni-ZnO monolayer as a resistance-type gas sensor, while the charge-transfer analysis in the electric field indicates its potential as a field-effect transistor gas sensor.

Our calculations expound the possible application of the Ni-ZnO monolayer in the sensing field and can stimulate the study on adsorption and sensing behaviors of the TM-ZnO monolayer in the near future.

4. COMPUTATIONAL DETAILS

In this project, all calculations were implemented in the Dmol$^3$ package, where the generalized gradient approximation (GGA) and the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional with Semicore Pseudopots treatment were adopted. The DFT-D2 method proposed by Grimme was employed to understand the van der Waals force and long-range interactions. Double numerical plus polarization (DNP) was used as the atomic orbital basis set. The Brillouin zone with k-point mesh of $7 \times 7 \times 1$ in a Monkhorst–Pack grid was set for both geometric optimizations and electronic calculations. The k-point test for the Ni-ZnO monolayer is listed in Table S1, which indicates the good accuracy of the k-point selected in this work. The energy tolerance accuracy of $10^{-5}$ Ha, maximum force of $2 \times 10^{-3}$ Ha/Å, and displacement of 5.0 Å were defined for geometric optimization, while the self-consistent loop energy of $10^{-6}$ Ha and global orbital cutoff radius and smearing of 0.005 Ha were defined for electronic calculations, which guarantee the high accuracy of the obtained total energy of every system.

We established a 4 x 4 x 1 supercell for the pristine ZnO monolayer, which contains 16 Zn and 16 O atoms to conduct the calculations in this work. The vacuum region was set to 15 Å to prevent the possible interaction between adjacent units. Furthermore, Hirshfeld analysis was considered to analyze the atomic charge of the Ni dopant ($Q_{Ni}$) in the doping system and the molecular charge of the adsorbed gas ($Q_{T}$) in the gas adsorption systems.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acsomega.0c03663.

Total energy of the Ni-ZnO monolayer with varying k-points (PDF)

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Notes

The author declares no competing financial interest.

ACKNOWLEDGMENTS

This research work was funded by the Chongqing Natural Science Foundation (no. cstc2019jcylxmsxmX0772) and the Key Talents Project of Chongqing Industrial Polytechnic College (no. GZY2018GGRC-34).

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