Adsorption Property of CS$_2$ and COF$_2$ on Nitrogen-Doped Anatase TiO$_2$(101) Surfaces: A DFT Study
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ABSTRACT: SF$_6$ has been utilized widely as an electrical insulation medium because of its excellent arc extinguishing performance and insulation characteristics. In this paper, the adsorption property of two kinds of key SF$_6$ carbon-containing decomposition components (CS$_2$ and COF$_2$) on nitrogen-doped anatase TiO$_2$(101) (N–TiO$_2$) surfaces was simulated and analyzed based on density functional theory. The results demonstrated that N–TiO$_2$ shows good gas sensitivity toward CS$_2$ with the increase of conductivity but is insensitive toward COF$_2$. In addition, the gas-sensing property of CS$_2$ on N–TiO$_2$ is stronger than that of COF$_2$. This work provides the theoretical information on such a gas-sensitive material for key SF$_6$ carbon-containing decomposition components, supporting its utilization as a chemical sensor applied in condition monitoring and defect diagnosis in SF$_6$ gas-insulated equipment based on decomposition component analysis.

1. INTRODUCTION
SF$_6$ has been utilized widely in electrical equipment$^{1-6}$ because of its excellent arc extinguishing performance and insulation characteristics.$^{7-9}$ However, harmful insulation defects are inevitably generated in the production, transportation, installation, and operation via vibration, mechanical friction, collision, and other factors. Moreover, such insulation defects would cause partial discharge (PD), which is also the mark of insulation defects. However, the withstand voltage of the equipment would considerably decrease without the defects not handled in time.$^{10,11}$

Under the action of PD, the SF$_6$ gas molecule would decompose to the primary decomposition products, namely, SF$_6$, SF$_5$, SF$_4$, F$_2$, and F, which will react chemically with trace H$_2$O, trace O$_2$, metal vapor, and organic solid insulation materials in the gas chamber of gas-insulated equipment to generate stable products including SOF$_2$, H$_2$S, SOF$_2$, SO$_2$F$_2$, CS$_2$, C$_2$F$_6$, CF$_3$, HF, COF$_2$, and so on.$^{12-14}$ The method of condition monitoring and defect diagnosis in SF$_6$ gas-insulated equipment based on decomposition component analysis (DCA) is an advantageous technique owing to its high sensitivity and capability to identify the fault type, without being affected by electromagnetic interference.$^{15-17}$

With a remarkably high catalytic property, TiO$_2$(101) nanotubes with good surface thermodynamic stability$^{3}$ have attracted considerable interest as gas sensors.$^{18,19}$ Noble metal doping of TiO$_2$ can improve the gas-sensing ability for specific gases.$^{20-22}$ Currently, the nitrogen-doped anatase TiO$_2$ (N–TiO$_2$) nanotube for photocatalytic activity has been studied.$^{23-26}$ The literature$^{27}$ reported the detection of SF$_6$ sulfur-containing decomposition components, namely, SOF$_2$, SO$_2$F$_2$, and SO$_2$ by N-doped anatase TiO$_2$. However, there are few studies about the adsorption of SF$_6$ carbon-containing decomposition components on the N–TiO$_2$ nanotube material, especially some key SF$_6$ decomposition components, namely, CS$_2$ and COF$_2$. The amounts of CS$_2$ and COF$_2$ could reach 12 and 80 μL/L, respectively, during the operation of gas electrical equipment. They are related to solid insulators and can more effectively represent the type and degree of solid insulator defect in gas-insulated equipment.$^{28-31}$ Consequently, this paper focuses on the gas sensitivity of N–TiO$_2$ on CS$_2$ and COF$_2$. Some parameters of the adsorption property were simulated and analyzed. This work provides the fundamental gas sensitivity information on TiO$_2$ nanotubes as the chemical sensors applied in condition monitoring and defect diagnosis in SF$_6$ gas-insulated equipment based on DCA.

2. COMPUTATION DETAILS
The simulation was implemented in Materials Studio with the DMol3 module based on the density functional theory (DFT).$^{32}$ The supersize of the N–TiO$_2$(101) surface is 10.88 1011.33 1.19 Å with a 12 Å vacuum layer. The composition of the N dopant is 0.833%. The Perdew–Burke–Ernzerhof functional generalized gradient approximation was utilized to deal with the electron exchange and correlation.$^{33}$ The maximum force,
energy tolerance accuracy, and maximum atom displacement were selected as 0.002 Ha/Å, 1.0 $10^{-5}$ Ha, and 5 $10^{-3}$ Å, respectively. The k-point of the Monkhorst-Pack grid was sampled to $2 \times 2 \times 1$ of the Brillouin zone. The charge density convergence accuracy of the self-consistent field was 1.0 $10^{-6}$ Ha. The Grimme method (DFT-D) was utilized for a better considering of the dispersion forces or van der Waals interactions. A smearing of 0.005 Ha was employed to ensure the accurate results of total energy. In addition, the atomic orbital basis set was the double numerical plus polarization (DNP).

The adsorption energy $E_d$ for a gas molecule adsorption system was as shown in formula 1

$$E_d = E_{gas+sur} - E_{gas} - E_{sur}$$

(1)

where $E_{gas+sur}$, $E_{gas}$, and $E_{sur}$ represent the total system energy after gas molecule adsorption, the energy of individual gas molecules, and the energy of the isolated TiO$_2$ surface, respectively. If $E_d > 0$, extra energy is required for the process of gas adsorption on the TiO$_2$ surface, which could not happen spontaneously and vice versa.

The electron population in the process of adsorption was calculated via Mulliken charge population analysis. If the Mulliken charge population $Q_d > 0$, it denotes that the gas molecules donated electrons to the TiO$_2$ surface during the process.

3. RESULTS AND DISCUSSION

3.1. Model Analysis of N–TiO$_2$ and Gas Molecules.

Many research studies show that the doping of TiO$_2$ can improve the gas-sensing ability significantly. The geometric structures of CS$_2$, COF$_2$, and N–TiO$_2$ are optimized before the simulation of the adsorption process and shown in Figure 1, where the parameters of bond length and bond angle are in Å and °, respectively. Figure 1a,b shows the optimized structures of the CS$_2$ and COF$_2$ gas molecules, where the bond length of C–S in CS$_2$ is 1.571 Å. The bond lengths of C–O and C–F in COF$_2$ are 1.185 and 1.337 Å, respectively. The doping position of the N atom is based on the previous studies, that is, one oxygen atom on the surface is replaced with a nitrogen atom. The new nitrogen atom and titanium atom form the bond Ti–N.

The comparison of the density of states (DOS) distribution between native TiO$_2$ and nitrogen-doped TiO$_2$ is shown in Figure 1d. One can observe that the energy gap decreases, to a large scale, after doping nitrogen on anatase TiO$_2$(101) surfaces. This means that the electrons in the valence band would be easier to move to the conduction band and enhance the gas-sensing ability.

3.2. Adsorption Property of CS$_2$ and COF$_2$ on N–TiO$_2$.

The optimized model and parameters (adsorption energy, adsorption distance, and Mulliken population analysis) of CS$_2$ and COF$_2$ on the N–TiO$_2$ surface are shown in Figures 2 and 3 and Table 1. As for CS$_2$, there are two adsorption modes which were considered. The electrons of 0.005 e transfer from CS$_2$ molecules to the N–TiO$_2$ surface in the S atom-oriented system, that is, CS$_2$ approaches N–TiO$_2$ by the S atom. Moreover, the...
bond angle changes from 180 to $150.065^\circ$ and the bond length changes to 1.635 and 1.583 Å. However, in the C atom-oriented system, N$\rightarrow$TiO$_2$ acts as the electron donor. Moreover, the bond angle changes from 180 to $78.634^\circ$ and the bond length changes to 1.779 and 1.749 Å. For the two adsorption modes of CS$_2$, the adsorption distances are 1.253 and 1.696 Å, respectively, and the adsorption energies are $-1.188$ and $-2.394$ eV, respectively, implying that the energy is released in the adsorption process. Therefore, considering the above comparison, it

| gas | calculation system | adsorption energy (eV) | adsorption distance (Å) | charge transfer (e) |
|-----|-------------------|------------------------|------------------------|-------------------|
| CS$_2$ | S | $-2.394$ | 1.696 | 0.005 |
| | C | $-1.188$ | 1.253 | $-0.003$ |
| COF$_2$ | F | $-0.116$ | 3.096 | 0.002 |
| | O | $-0.616$ | 3.211 | $-0.002$ |
| | C | $-0.273$ | 2.772 | 0.006 |

Figure 3. Adsorption configuration of COF$_2$ on the N-doped TiO$_2$(101) surface. (a) C atom-oriented system, (b) F atom-oriented system, and (c) O atom-oriented system.

Table 1. Adsorption Parameters of CS$_2$ and COF$_2$ on the N$\rightarrow$TiO$_2$ Nanotube Surface

Figure 4. DOS of CS$_2$ on the N-doped TiO$_2$(101) surface. (a) DOS of the S atom-oriented system, (b) p orbital DOS of the S atom-oriented system, (c) DOS of the C atom-oriented system, and (d) p orbital DOS of the C atom-oriented system.
could be easier for CS$_2$ to adsorb on the N–TiO$_2$ surface by the S atom.

As for COF$_2$, there are three adsorption modes which were considered, namely, the C atom-, F atom-, and O atom-oriented systems. All the bond angles and lengths of COF$_2$ have small changes after adsorption in the three adsorption modes. In the C atom-oriented system, the COF$_2$ gas molecule donates electrons of 0.006 e, and the adsorption distance and energy are 2.772 Å and $-0.273$ eV, respectively. In the F atom-oriented system, the calculation adsorption distance and energy are 3.096 Å and $-0.116$ eV, respectively, and the gas molecule donates a few of electrons of 0.002 e. The final adsorption structure of COF$_2$ approaching the N–TiO$_2$ surface by the O atom is shown in Figure 3c. The calculation adsorption distance and energy in the O atom-oriented system are the largest in the three kinds of adsorption modes. Meanwhile, the gas molecule acts as the charge recipient. The comparison of the three adsorption modes shows that it could be easier for COF$_2$ to adsorb on the N–TiO$_2$ surface by the O atom. In addition, all the adsorption energies of COF$_2$ on N–TiO$_2$ are markedly smaller than those of CS$_2$ on N–TiO$_2$, which suggests that the adsorption effect of CS$_2$ on N–TiO$_2$ is quite stronger and there is a more stable adsorption structure.

Figure 5. DOS of COF$_2$ on the N-doped TiO$_2$(101) surface. (a) DOS of the F atom-oriented system, (b) p orbital DOS of the F atom-oriented system, (c) DOS of the O atom-oriented system, (d) p orbital DOS of the O atom-oriented system, (e) DOS of the C atom-oriented system, and (f) p orbital DOS of the C atom-oriented system.
The DOS of CS$_2$ on the N-doped TiO$_2$ surface is shown in Figure 4. Compared with the DOS of the isolated N–TiO$_2$ surface, both the DOS of the S atom-oriented system and the DOS of the C atom-oriented system are shifted to the right significantly. There appear two novel peaks in the DOS distribution of the S atom-oriented system around $-16$ and $-8$ eV in comparison with that of isolated N–TiO$_2$ and one novel peak in the DOS distribution of the C atom-oriented system around $-8$ eV in comparison to that of isolated N–TiO$_2$. Considering that the pseudogap of the S atom-oriented system is wider than that of the C atom-oriented system, the interaction between the S atom and N-doped TiO$_2$ surface is stronger, which confirms the previous conclusion. In addition, the $p$ orbital of the CS$_2$ gas molecule contributes the largest to the DOS of CS$_2$ gas molecules, which is also shown in Figure 4b,d, and one can find that the $p$ orbital DOS of the S atom-oriented system and the C atom-oriented system is similar to their total DOS, respectively.

The DOS distribution of COF$_2$ on the N-doped TiO$_2$ surface is shown in Figure 5. It could confirm that the weak interaction between COF$_2$ and the N–TiO$_2$ surface by the comparison of the C atom-, O atom-, and F atom-oriented systems with isolated N–TiO$_2$ in Figure 5a,c,e, where three DOS distributions are basically overlapped at the area near the Fermi level and the range between $-20$ and $-15$ eV. Moreover, the only change between the DOS distribution of the COF$_2$ system and that of isolated N–TiO$_2$ are four new peaks in the F atom- and C atom-oriented systems and two new peaks in the O atom-oriented systems between $-11$ and $-7$ eV. The pseudogaps of the C atom-, O atom-, and F atom-oriented systems are similar. In addition, the DOS and $p$ orbital of COF$_2$ gas molecule distributions are also shown in Figure 5b,d,f.

The frontier molecular orbital theory is employed to explore the conductivity of the N-doped TiO$_2$(101) surface via gas adsorption. The distributions of the highest occupied molecular orbital (HOMO) and their energies, lowest unoccupied molecular orbital (LUMO) and their energies, and the energy gap $E_g$ ($E_g = E_{\text{LUMO}} - E_{\text{HOMO}}$) are shown in Figure 6.
One can observe that the energies of the HOMO and LUMO of isolated N–TiO₂ are −7.451 and −5.723 eV, respectively, with an E₀ of 1.728 eV. As for the CS₂ adsorption, the HOMO and LUMO are redistributed evidently. The energies of the HOMO and LUMO of the S atom-oriented system are −4.951 and −4.918 eV, respectively, in Figure 6b1, which are lower than those of isolated N–TiO₂. Moreover, the energy gap (0.033 eV) of the S atom-oriented system decreases remarkably in comparison to that of isolated N–TiO₂.

The molecular orbital distribution of the C atom-oriented system is shown in Figure 6b2, where the energies of the HOMO and LUMO are −4.674 and −4.653 eV, respectively, and the energy gap E₀ surprisingly decreases to 0.021 eV. Consequently, both the energy gaps of the S atom- and C atom-oriented systems when CS₂ adsorbs on N– TiO₂ are much lower than that of isolated N–TiO₂, leading to electrons in the valence band to easily jump to the conduction band. Therefore, it can be assumed that to a large scale, the conductivity of N–TiO₂ would be increased after adsorbing CS₂.

In Figure 6c, the orbital distributions of the HOMO and LUMO for COF₂ adsorption are exhibited. One can observe that COF₂ contributes less to the orbital distributions in comparison to N–TiO₂. In addition, the energies of the HOMO in the F atom-, O atom-, and C atom-oriented systems are −7.452, −7.373, and −7.478 eV, respectively, and the energies of the LUMO in the F atom-, O atom-, and C atom-oriented systems are −5.718, −5.662, and −5.750 eV, respectively. Consequently, all the energy gaps for COF₂ adsorption are similar to that of isolated N–TiO₂, denoting that the conductivity of N–TiO₂ would be slightly changed after adsorbing COF₂.

In summary, it can be concluded that N-doped TiO₂ is a desirable material to detect CS₂ gas based on the increased conductivity and stable adsorption structure. However, because of the small conductivity change and low adsorption energies, this material is probably not suitable for detecting the presence of COF₂ precisely. Therefore, it could be hypothesized that the material can function as a sensor in the application of condition monitoring and defect diagnosis in SF₆ gas-insulated equipment based on DCA.

4. CONCLUSIONS

In this paper, the parameters of adsorption property, namely, adsorption energy, distance, DOS, and frontier molecular orbital theory, were simulated and analyzed for comprehensively investigating the gas sensitivity of N-doped anatase TiO₂(101) on two kinds of SF₆ carbon-containing decomposition components, CS₂ and COF₂, based on DFT. The results manifest the following:

(1) The main adsorption positions for CS₂ on the N–TiO₂ surface are probably by the S atom. However, the N–TiO₂ surface adsorbing COF₂ is probably by the O atom. The gas-sensing property of CS₂ on N–TiO₂ is quite stronger than that of COF₂. In addition, there is less charge transfer in both the CS₂ and COF₂ adsorption processes.

(2) The simulation and analysis results of DOS and frontier molecular orbital theory consistently indicate that the N–TiO₂ surface has good sensitivity to the CS₂ gas molecule because of the increase of conductivity but exhibits insensitivity toward the COF₂ gas molecule.

This work provides theoretical information on such a gas-sensitive material for SF₆ carbon-containing decomposition components, which could function as a sensor in the application of condition monitoring and defect diagnosis in SF₆ gas-insulated equipment based on DCA.

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