Rh-doped MoTe$_2$ Monolayer as a Promising Candidate for Sensing and Scavenging SF$_6$ Decomposed Species: a DFT Study

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Abstract

In this work, the adsorption and sensing behaviors of Rh-doped MoTe$_2$ (Rh-MoTe$_2$) monolayer upon SO$_2$, SOF$_2$, and SOF$_2$F$_2$ are investigated using first-principles theory, wherein the Rh doping behavior on the pure MoTe$_2$ surface is included as well. Results indicate that $T_{Mo}$ is the preferred Rh doping site with $E_b$ of $-2.69$ eV, and on the Rh-MoTe$_2$ surface, SO$_2$ and SOF$_2$ are identified as chemisorption with $E_{ad}$ of $-2.12$ and $-1.65$ eV, respectively, while SOF$_2$F$_2$ is physically adsorbed with $E_{ad}$ of $-0.46$ eV. The DOS analysis verifies the adsorption performance and illustrates the electronic behavior of Rh doping on gas adsorption. Band structure and frontier molecular orbital analysis provide the basic sensing mechanism of Rh-MoTe$_2$ monolayer as a resistance-type sensor. The recovery behavior supports the potential of Rh-doped surface as a reusable SO$_2$ sensor and suggests its exploration as a gas scavenger for removal of SOF$_2$ in SF$_6$ insulation devices. The dielectric function manifests that Rh-MoTe$_2$ monolayer is a promising optical sensor for selective detection of three gases. This work is beneficial to explore Rh-MoTe$_2$ monolayer as a sensing material or a gas adsorbent to guarantee the safe operation of SF$_6$ insulation devices in an easy and high-efficiency manner.

Keywords: Rh-MoTe$_2$ monolayer, First-principles theory, SF$_6$ decomposed species, Gas sensor

Introduction

SF$_6$ insulation devices, in high even ultra-high voltage power systems, are one kind of the most important and expensive equipment [1–3], except electrical transformers [4, 5], to guarantee the safe operation of the whole system. These contributions attribute to the strong arc-extinguishing property and high electronegativity of SF$_6$ gas that behaves as an insulation media in such devices [6]. However, in a long-running one, SF$_6$ could still be decomposed into several low-fluorine sulfides by the power of partial discharge caused by inevitable inner defects of the equipment [7, 8]. Moreover, these by-products will further interact with the surrounding trace water and oxygen, forming some stable chemicals such as SO$_2$, SOF$_2$, and SOF$_2$F$_2$ and instead deteriorating the insulation behavior of SF$_6$ [9]. Therefore, detecting these decomposed species has been regarded as an effective manner to evaluate the decomposing status of SF$_6$ and to reflect the operation status of related insulation devices [10].

With the growing attention of transition metal dichalcogenides (TMDs), MoS$_2$-based sensors have been proposed for detection of SF$_6$ decomposed species [11–13]. These reports have demonstrated the appropriateness and superiority of transition metal (TM)-doped MoS$_2$ monolayer for sensing components including SO$_2$ and SOF$_2$. Besides, a theoretical study on the sensing characteristic of pristine MoTe$_2$ monolayer upon SF$_6$ decomposed species proves its suitability for sensing SO$_2$ [14]. Moreover, recent advancements in chemical vapor...
deposition (CVD) used for large-scale synthesis of TMDs largely accelerate the development of MoTe$_2$ monolayer for gas sensing applications [15–17]. As reported, MoTe$_2$ monolayer possesses outstanding carrier mobility, large bond length, and low binding energy, which provides it with high sensitivity upon gas interactions at room temperature [18]. Thus, it is hopeful that MoTe$_2$ monolayer is quite a promising candidate for gas sensing, and its application for detection of SF$_6$ decomposed species should be further explored.

It is well proved that TM-doped 2D nanomaterials possess stronger adsorption performance and sensing behavior upon gaseous molecules compared with pristine surfaces [19–22]. This is because of the admirable chemical activity and catalytic behavior of TM whose d orbital can strongly hybridize with those adsorbed molecules, facilitating the chemisorption and enlarging the orbital can strongly hybridize with those adsorbed molecules, facilitating the chemisorption and enlarging the charge transfer [23–25]. When it comes to the MoTe$_2$ monolayer, to the best of our knowledge there have few theoretical reports on the TM-doping behavior on its monolayer; meanwhile, related adsorption and sensing behaviors of TM-doped MoTe$_2$ monolayer upon gases are also less explored. Among the TM elements, rhodium (Rh) with strong catalytic performance has been demonstrated as a desirable TM dopant on other nanosurfaces for gas adsorption [26, 27]. Especially, ref. [26] investigates the Rh doping behavior on the MoSe$_2$ monolayer and its enhanced performance for toxic gas adsorption. From this regard, it would be interesting using the first-principles theory to study the Rh doping behavior on the less explored MoTe$_2$ monolayer to compare their geometric property and give a better understanding of Rh doping on the TMDs. Beyond that, the adsorption and sensing performances of Rh-doped MoTe$_2$ (Rh-MoTe$_2$) monolayer upon three SF$_6$ decomposed species, namely, SO$_2$, SOF$_2$, and SO$_2$F$_2$, were theoretically simulated as well to explore its potential sensing application in some typical areas. The electronic and optical behaviors of Rh-MoTe$_2$ monolayer upon gas adsorption provide the basic sensing mechanisms for its exploration as a resistance-type or optical gas sensor to realize the detection of SF$_6$ decomposed species. The desorption behavior verifies the potential of Rh-MoTe$_2$ monolayer as a gas scavenger to remove these noxious gases in SF$_6$ insulation devices, which from another aspect guarantees the safe operation of the power system. This work would be meaningful to propose novel nanosensing material and its application for evaluating the operation status of SF$_6$ insulation devices in an easy and high-efficiency manner.

**Computational Details**

All the results were obtained in the Dmol$^3$ package [28] based on the first-principles theory. The DFT-D method proposed by Grimme was adopted [29] to better understand the van der Waals force and long-range interactions. Perdew-Burke-Ernzerhof (PBE) function with generalized gradient approximation (GGA) was employed to treat the electron exchange and correlation terms [30]. Double numerical plus polarization (DNP) was employed as the atomic orbital basis set [31]. The Monkhorst-Pack k-point mesh of $7 \times 7 \times 1$ was defined for supercell geometry optimizations, while a more accurate k-point of $10 \times 10 \times 1$ was selected for electronic structure calculations [32]. The energy tolerance accuracy, maximum force, and displacement were selected as $10^{-5}$ Ha, $2 \times 10^{-3}$ Ha/Å, and $5 \times 10^{-5}$ Å [33], respectively. For static electronic structure calculations, self-consistent loop energy of $10^{-6}$ Ha, the global orbital cut-off radius of 5.0 Å to ensure the accurate results of total energy [34].

A MoTe$_2$ monolayer with supercell of $4 \times 4$ and vacuum region of 15 Å containing 16 Mo and 32 Te atoms was established to perform the whole calculation below. It has been proved that a $4 \times 4$ supercell is large enough to conduct the gas adsorption process while a 15 Å slab is proper to prevent the interaction between adjacent units [35]. Apart from that, the Hirshfeld method [36] was employed throughout this work to analyze the atomic charge of Rh dopant ($Q_{Rh}$) and molecular charge of adsorbed molecules ($Q_T$). Therefore, a positive value of $Q_{Rh}$ represents the Rh dopant (gas molecule) as an electron donor, while a negative $Q_{Rh}$ or $Q_T$ indicates the related electron-accepting behavior. Only the most favorable configurations of Rh-MoTe$_2$ monolayer and adsorption systems are plotted and analyzed in the following parts.

**Results and Discussion**

**Analysis of Rh-MoTe$_2$ Monolayer**

Upon Rh-MoTe$_2$ monolayer, four possible adsorption sites are considered, traced as $T_{Mo}$ (at the top of the Mo atom), $T_{Te}$ (at the top of Te atom), and $T_{B}$ (the bridge site between two Te atoms), respectively. The binding energy ($E_b$) for Rh doping onto the MoTe$_2$ monolayer is formulated as:

$$E_b = E_{Rh-MoTe_2} - E_{Rh} - E_{MoTe_2},$$

where $E_{Rh-MoTe_2}$, $E_{Rh}$, and $E_{MoTe_2}$ represent the energies of the Rh-MoTe$_2$ monolayer, Rh atoms, and pristine MoTe$_2$ monolayer, respectively.

Based on this definition, the most stable configuration (MSC) with the lowest $E_b$ in line with related electron deformation density (EDD) of Rh-MoTe$_2$ monolayer is depicted in Fig. 1. One can see that the Rh dopant is trapped on the $T_{Mo}$ site, forming three covalent bonds.
with neighboring Te atoms on the upper layer of MoTe$_2$ monolayer. Three Rh-Te bonds are measured equally as 2.54 Å, shorter than the sum of covalent radii of Rh and Te atoms (2.61 Å [37]), indicating the formation of chemical bonds for Rh doping on the MoTe$_2$ layer. The calculated $E_b$ of this configuration is $-2.69$ eV, much larger than those of $-2.14$ eV for T$_H$ site, $-1.28$ eV for T$_Te$ site, and $-2.55$ eV for T$_B$ site. It is worth noting that the Rh-Te bonds in Rh-MoTe$_2$ monolayer are longer than those of Rh-Se bonds in Rh-MoSe$_2$ monolayer and the $E_b$ for Rh doping is smaller on the MoTe$_2$ surface in comparison with that of MoSe$_2$ counterpart. These indicate the stronger binding force of Rh-Se than Rh-Te bonds. Based on the Hirshfeld method, the Rh dopant behaves as an electron acceptor during doping process, which receives 0.045 e from the MoTe$_2$ surface proving its electron-accepting behavior in surface doping [26].

This is in accordance with the EDD in which the Rh atom is mainly surrounded by electron accumulation.

The band structure (BS) and density of state (DOS) of Rh-MoTe$_2$ system are depicted in Fig. 2 to better understand the caused change in electronic behavior of MoTe$_2$ surface by Rh doping. It is reported that pristine MoTe$_2$ monolayer has a direct bandgap of 1.10 eV [38]. In Fig. 2a, the bandgap of Rh-MoTe$_2$ monolayer is obtained as 0.937 eV according to the calculations. This indicates that the Rh dopant induces several impurity states within the bandgap of MoTe$_2$ system, narrowing the bandgap of the whole system accordingly. Besides, the top of the valence band is localized on the $\Gamma$ point and the bottom of the conduction band is on the $K$ point, implying the indirect semiconducting property for Rh-MoTe$_2$ system. In Fig. 2b, it is seen that the states of Rh dopant contribute largely to the top of the conduction

![Fig. 1](image1)

![Fig. 2](image2)
band of pristine MoTe$_2$ monolayer and forming several novel DOS peaks around the Fermi level. These peaks seemingly change the electronic behavior of the whole system, reducing its electrical conductivity accordingly. Because the Rh dopant is trapped on the T$_{Mo}$ site forming bonds with Te atoms, the atomic DOS of Rh and Te atoms are plotted to understand the electron hybridization behavior between them. As shown in Fig. 2c, the Rh 4$d$ orbital is strongly hybrid with the Te 5$p$ orbital from −5 to 2 eV, accounting for the significant bonding interaction that leads to the formation of chemical bonds of Rh-Te.

Gas Adsorption Configurations of Rh-MoTe$_2$ Monolayer

Based on the relaxed structure of Rh-MoTe$_2$ monolayer, the adsorption of SO$_2$, SOF$_2$, and SO$_2$F$_2$ molecules onto its surface around the Rh center are fully simulated. Before that, the geometric structures of the three gas molecules should also be optimized as well, as exhibited in Additional file 1: Figure S1. The adsorption energy ($E_{ad}$) is used to determine the most stable configuration of each system, formulated as:

$$E_{ad} = E_{Rh-MoTe_2/gas} - E_{Rh-MoTe_2} - E_{gas}$$

in which the $E_{Rh-MoTe_2/gas}$ and $E_{Rh-MoTe_2}$ are the total energy of Rh-MoTe$_2$ monolayer before and after adsorption, whereas $E_{gas}$ is the energy of isolated gas molecule. According to this definition, the MSC with the lowest $E_{ad}$ could be identified.

To better understand the charge-transfer behavior during gas adsorption, EDD is also calculated for each configuration. Detailed information for SO$_2$, SOF$_2$, and SO$_2$F$_2$ adsorption could be seen in Figs. 3, 4, and 5, respectively. In addition, the adsorption parameters including $E_{ad}$, charge-transfer ($Q_T$), and bond length ($D$) are listed in Table 1.

For SO$_2$ adsorption on the Rh-MoTe$_2$ monolayer, one can find from Fig. 3 that the SO$_2$ molecule is basically parallel to the MoTe$_2$ layer with one O atom and one S atom trapped by the Rh dopant. As listed in Table 1, the newly formed Rh-O and Rh-S bonds are measured as 2.16 and 2.36 Å, respectively, indicating the strong binding force between Rh dopant and SO$_2$ molecule. Besides, the $E_{ad}$ is obtained as −1.65 eV implying the chemisorption for the SO$_2$ system, and the $Q_T$ is obtained as −0.333 e implying the electron-withdrawing behavior of SO$_2$. After adsorption, the Rh dopant is negatively charged by 0.017 e, which means it contributes 0.028 e to the adsorbed SO$_2$ and the other part of charge (0.305) comes from the MoTe$_2$ monolayer. Compared with the adsorption parameters in the MoTe$_2$/SO$_2$ system ($E_{ad} = −0.245$ eV; $Q_T = −0.086$ e; $D = 3.44$ Å [14]), one can infer that Rh doping largely enhances the reacting behavior and electronic redistribution for the MoTe$_2$ monolayer upon SO$_2$ adsorption, making the adsorbent much desirable for gas interaction. Moreover, the S-O bonds in the SO$_2$ molecule are separately elongated to 1.50 and 1.58 Å after adsorption, from that uniform 1.48 Å in the gas phase; the three Rh-Te bonds in the Rh-MoTe$_2$ monolayer are elongated to 2.58, 2.58, and 2.64 Å, respectively. These deformations imply the geometric activation during adsorption for both nano-adsorbent and gaseous adsorbate, which further confirms the strong chemisorption here. From the EDD distribution, it is found that the SO$_2$ molecule is surrounded by electron accumulation, which agrees with the Hirshfeld analysis; and electron accumulation largely surrounds the

![Fig. 3](image_url) MSC (a) and EDD (b) of Rh-MoTe$_2$/SO$_2$ system. In EDD, the green (rosy) areas indicate electron accumulation (depletion), with isosurface as 0.005 e/Å$^3$. 
Rh-S and Rh-O bonds, suggesting the electron hybridization in the formation of new chemical bonds.

In the Rh-MoTe$_2$/SOF$_2$ system presented in Fig. 4, the SOF$_2$ molecule preferred to approach the Rh dopant by the O-end position and the plane made of the S atom and two F atoms are almost parallel to the MoTe$_2$ layer. However, there has no obvious evidence suggesting the formation of new bonds between Rh dopant and SOF$_2$ molecule. The nearest distance of Rh-O is measured to be 2.25 Å, a little longer than that in the SO$_2$ system, and the SOF$_2$ molecule does not undergo large geometric deformation after interaction. These findings manifest the relatively weaker adsorption performance of Rh-MoTe$_2$ monolayer upon SOF$_2$ in comparison with SO$_2$.

As presented in Table 1, the $E_{\text{ad}}$ is calculated as $-0.46$ eV supporting the physisorption again [39] and the $Q_T$ is obtained as 0.040 e implying the electron-donating behavior of SOF$_2$. According to the EDD, one can see that the electron accumulation is mainly localized on the area between the SOF$_2$ molecule and Rh dopant, which implies somewhat hybridization between them, while the electron depletion on the SOF$_2$ molecule agrees with the Hirshfeld analysis.

In terms of the SO$_2$F$_2$ adsorption system, as depicted in Fig. 5, it is found that after optimization, the SO$_2$F$_2$ molecule tends to be resolved to be a F atom and a SO$_2$F group. Both are captured by the Rh dopant forming a Rh-F bond and a Rh-S bond, respectively, with
related bond length of 2.02 and 2.26 Å. The newly formed bonds indicate the strong binding force between Rh dopant and SO$_2$F$_2$ molecule, which combined with the calculated $E_{ad}$ of 2.12 eV evidence the chemisorption nature for Rh-doped surface upon SO$_2$F$_2$ adsorption, similar as that in the SO$_2$ system. From the EDD, the electron accumulation is significantly localized on the SO$_2$F$_2$ molecule, in agreement with the result of $Q_T$ (~0.753 e) based on Hirshfeld analysis. On the other hand, a large number of electron depletion is localized on the Rh dopant and a little is on the MoTe$_2$ monolayer. In other words, the Rh dopant contributes largely to the charge-transfer to the adsorbed SO$_2$F$_2$ molecule, manifesting its high electron mobility and strong chemical reactivity [40]. At the same time, the overlap of electron accumulation and electron depletion on the Rh-S and Rh-F bonds suggest the electron hybridization in their formation.

Based on the analysis of adsorption configuration and parameters, one can conclude that the Rh-MoTe$_2$ monolayer possesses the best performance upon SO$_2$F$_2$ molecule, followed by SO$_2$ and the last one comes to SOF$_2$. In the meanwhile, the Rh dopant can largely affect the electron distribution of this system and therefore dramatically alter the electronic behavior of the Rh-MoTe$_2$ monolayer.

**Electronic Behaviors of Rh-MoTe$_2$ Monolayer upon Gas Adsorption**

The band structure (BS) and density of state (DOS) of three adsorption systems are exhibited in Fig. 6 to comprehend the electronic behavior of Rh-MoTe$_2$ monolayer in gas adsorption. As above analyzed, Rh-MoTe$_2$ monolayer has the best performance upon SO$_2$F$_2$ adsorption. Thus, from Fig. 6 (c2), it is seen that the molecular DOS of SO$_2$F$_2$ experiences pronounced deformations, which is integrally left-shifted and some of the states combine to a large one below the Fermi level. From Fig. 6 (c3) where the orbital DOS is shown, it is seen that the Rh 4$d$ orbital is highly hybrid with the F 2$p$ orbital, and is somewhat hybrid with S 3$p$ orbital. From this aspect, it is presumed that Rh-F bond is stronger than that of Rh-S. In the SO$_2$ system, the Rh 4$d$ orbital is highly hybrid with the O 2$p$ orbital and followed by the S 3$p$ orbital in Fig. 6 (a3), and one could also presume that Rh dopant has stronger binding force with the O atom rather than the S atom. Due to such hybridization, the molecular DOS of SO$_2$ in Fig. 6 (a2) suffers remarkable deformation. As for the SOF$_2$ system, one can see in Fig. 6 (b3) that the Rh dopant has little orbital hybridization with the nearest O atom, which supports the weak interaction for SOF$_2$ adsorption.

Along with the change of orbital and molecular DOS, the whole state of the gas adsorbed system would be automatically changed compared with the pure Rh-MoTe$_2$ system. From Fig. 6 (a1)–(c1) where the BS of the adsorbed system are portrayed, one can see that the BS in the SOF$_2$ system does not experience significant deformation in comparison with that of isolated Rh-MoTe$_2$ system, while those in the SO$_2$ and SO$_2$F$_2$ system are different, in which some novel states are emerged around the Fermi level, thus narrowing the bandgap largely. Detailesly, the bandgap of the Rh-MoTe$_2$ is reduced to 0.863, 0.913, and 0.675 eV after adsorption of SO$_2$, SOF$_2$, and SO$_2$F$_2$, respectively. This provides the basic sensing mechanism for Rh-MoTe$_2$ monolayer as a possible resistance-type gas sensor.

**Frontier Molecular Orbital Analysis**

To confirm the results based on the BS analysis, the frontier molecular orbital theory is performed to analyze the distribution and energies of frontier molecular orbitals (FMO) of isolated and gas adsorbed Rh-MoTe$_2$ surface. The FMO contains highest occupied molecular (HOMO) and lowest unoccupied molecular orbital (LUMO), and the energy gap between them can evaluate the electrical conductivity of the analyzed system [41]. To obtain the accurate results of the energies of FMO, the smearing in this part of calculations is set to $10^{-4}$ Å. The distributions and energies of FMO of Ru-MoTe$_2$ monolayer before and after gas adsorptions are described in Fig. 7.

From Fig. 7a, one can observe that the HOMO and LUMO are mainly localized at the Rh dopant, suggesting its high reactivity in the surroundings. The energies of HOMO and LUMO are obtained as ~4.885 and ~3.927 eV, respectively, with the calculated bandgap of 0.958 eV. After adsorption of three gas species, as seen in Fig. 7b–d, the FMO distributions of Rh-MoTe$_2$ surface are afflicted with different degrees of deformations, where the reaction occurs resulting in the convergence of the electron cloud. Along with these deformations, the energies of FMO have changed accordingly. It is found that the energies of FMO are decreased to different degrees after adsorption of three gases, in which those in SOF$_2$ system experience the largest decreases. However, the energy gap in SOF$_2$ system undergoes the smallest change in comparison with that of pure Rh-MoTe$_2$ system. Specifically, the energy gap of Rh-MoTe$_2$ monolayer (0.958 eV) is decreased by 0.044 eV after SOF$_2$
adsorption, while is reduced by 0.061 and 0.281 eV after \( \text{SO}_2 \) and \( \text{SO}_3 \text{F}_2 \) adsorption, respectively. These findings indicate that the electrical conductivity of Rh-MoTe\(_2\) monolayer will decrease after adsorption of three gases and the decrease is the most significant in the \( \text{SO}_3 \text{F}_2 \) system, which agree with the conclusions from BS analysis. Besides, the energy gaps from frontier molecular orbital theory is basically close to those of bandgaps from BS results, implying the good accuracy of our calculations.

**Sensing Response and Recovery Property**

The changes in the bandgap of Rh-MoTe\(_2\) monolayer after gas adsorption manifest its change in electrical conductivity in related gas atmosphere [42], which can provide the basic sensing mechanism for exploration of Rh-MoTe\(_2\) monolayer as a resistance-type gas sensor. Besides, the larger change in electrical conductivity would account for a higher sensitivity for gas detection. To identify the possibility of Ru-MoTe\(_2\) monolayer as a sensor, its conductivity \( \sigma \) and sensitivity \( S \) upon three typical gases are calculated using the following formulas [43, 44]:

\[
\sigma = A \cdot e^{-\frac{B_g}{kT}} \tag{3}
\]

\[
S = \frac{1}{\sigma_{\text{gas}}} - \frac{1}{\sigma_{\text{pure}}} = \frac{\sigma_{\text{pure}} - \sigma_{\text{gas}}}{\sigma_{\text{gas}}} \tag{4}
\]

In formula 3, \( A \) is a constant, \( B_g \) is the bandgap of the analyzed system, \( k \) is the Boltzmann constant, and \( T \) is
the working temperature. In formula 4, $\sigma_{\text{gas}}$ and $\sigma_{\text{pure}}$ respectively mean the conductivity of analyzed adsorption system and isolated Rh-MoTe$_2$ monolayer. According to such two formulas, it is found that the $S$ of certain surface could be obtained just with its bandgap before and after gas adsorption. After calculation, the sensitivities of Rh-MoTe$_2$ monolayer upon SO$_2$, SOF$_2$, and SO$_2$F$_2$ detection at 298 K are 76.3, 37.3, and 99.4%, respectively. These findings suggest that the Rh-MoTe$_2$ monolayer possess the most admirable sensing behavior upon

![Fig. 7 Distributions and energies of FMO in a Rh-MoTe$_2$ system, b SO$_2$ system, c SOF$_2$ system, and d SO$_2$F$_2$ system.](image)

![Fig. 8 Recovery time of Rh-MoTe$_2$ monolayer at various temperatures.](image)
SO$_2$F$_2$, followed by the SO$_2$ and the last one comes to SOF$_2$. This order is in accordance with those analysis of adsorption parameter and electronic behavior. Based on these results, it is hopeful that Rh-MoTe$_2$ monolayer could realize sensitive detection of SO$_2$ and SO$_2$F$_2$ at room temperature.

The recovery property is also important to evaluate the reusability of the gas sensor, and to reduce the recovery time ($\tau$) of gas desorption from certain surfaces, heating technique is usually considered since the recovery time is related to the temperature ($T$), formulated as $\tau = A^{-1}e^{(-E_a/K_BT)}$. In this formula, $A$ is the attempt frequency referring to $10^{12}$ s$^{-1}$ [46], $E_a$ is the potential barrier, determined as equivalent as $E_{ad}$ in this work, and $K_B$ is the Boltzmann constant ($8.318 \times 10^{-3}$ kJ/(mol·K)).

Based on the formula, the recovery behavior of Rh-MoTe$_2$ monolayer at 298, 448, and 598 K is portrayed in Fig. 8. It can be seen from this figure that the desorption of SO$_2$F$_2$ and SO$_2$ at room temperature are extremely difficult, while for SOF$_2$ the recovery time is quite short due to its weak binding force with the Rh-doped surface. Through heating, the recovery time for SO$_2$F$_2$ or SO$_2$ desorption is pronouncedly reduced, and when the temperature increases to 598 K, the recovery time in SO$_2$ system (79.48 s) becomes favorable which allow its reusability in several minutes. This supports the potential of Rh-MoTe$_2$ monolayer as a reusable gas sensor for detecting SO$_2$. On the other hand, the long recovery time for SO$_2$F$_2$ desorption at 598 K (7.24 × 10$^5$) also reflects the strong chemisorption here. Although continuing to increase the temperature can further reduce the recovery time, the thermostability of the sensing material and the high energy consumption in sensing application would be another problem. Given all these, Rh-MoTe$_2$ monolayer is not suitable as a sensor for SOF$_2$ detection. However, it provides us another thought to propose Rh-MoTe$_2$ monolayer as a gas adsorbent to scavenge this noxious gas in SF$_6$ insulation devices, thus guaranteeing their safe operation. Moreover, this part of analysis from another aspect reveals the inappropriateness to explore Rh-MoTe$_2$ monolayer as a SO$_2$F$_2$ sensor given the weak interaction with the surface.

**Optical Behavior of Rh-MoTe$_2$ Monolayer upon Gas Adsorption**

Given the desirable optical property of MoTe$_2$ monolayer, the calculation of the dielectric function of Rh-MoTe$_2$ monolayer upon gas adsorption is conducted, as displayed in Fig. 9, to illustrate its possibility as an optical gas sensor.

From Fig. 9, it is seen that there have three main adsorption peaks for the isolated Rh-MoTe$_2$ monolayer, localizing at 148, 389, and 1242 nm, among which the former two distance are in the range of ultraviolet ray and the last one is in the range of infrared ray. After gas...
adsorption, the peaks in ultraviolet range suffer small deformation and that in infrared range undergoes significant deformation. Detailedly, the peak intensity at 1242 nm decreases after SOF$_2$ adsorption whereas increases after SO$_2$ and SO$_2$F$_2$ adsorption, and the blue shift could also be identified in the SOF$_2$ system. Therefore, it could be assumed that Rh-MoTe$_2$ monolayer is a promising optical sensor for sensitive and selective detection of three gases by infrared device.

In short, it is worth adding that this work makes a progressive research for proposing novel nanomaterials to realize the detection of SF$_6$ decomposed species through various techniques, which would be significant to fulfill the evaluation of SF$_6$ insulation devices in an easy and high-efficiency manner.

### Conclusions

In this paper, the potential application of Rh-MoTe$_2$ monolayer as a gas sensor for detection of SF$_6$ decomposed species is explored, which mainly contains two aspects: (1) Rh doping behavior on the intrinsic MoTe$_2$ monolayer and (2) adsorption and sensing behaviors of Rh-MoTe$_2$ monolayer upon SO$_2$, SOF$_2$, and SO$_2$F$_2$. It is found that the Rh dopant prefers to be doped on the MoTe$_2$ surface through the T$_{Mo}$ site with $E_b$ of $\sim 2.69$ eV, exerting great electron hybridization with the Te atoms. The adsorption performance of Rh-MoTe$_2$ monolayer upon three gases are in order as SO$_2$F$_2 >$ SO$_2 >$ SOF$_2$, in which chemisorption is identified in SOF$_2$ and SO$_2$ systems while physisorption in SO$_2$F$_2$ system, as further supported by the DOS analysis. Rh-MoTe$_2$ monolayer is a promising resistance-type gas sensor for recycle detection of SO$_2$ with a response of 76.3%, is a desirable adsorbent for SO$_2$F$_2$ removal from the SF$_6$ insulation device, and is promising as an optical sensor for selective detection of three gases. All in all, Rh-MoTe$_2$ monolayer is a potential sensing material for detection of SF$_6$ decomposed species. This work is meaningful to propose novel nano-sensing material and to realize the effective evaluation of SF$_6$ insulation devices in an easy and high-efficiency manner.

### Methods Section

This work means to explore novel 2D sensing materials using first-principle theory for application in electrical engineering, through detecting the SF$_6$ decomposed species to evaluate the operation status of high-voltage insulation devices.

### Supplementary information

Supplementary information accompanies this paper at https://doi.org/10.1186/s11671-020-03361-6.
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