First-Principles Insight into a Ru-Doped SnS₂ Monolayer as a Promising Biosensor for Exhale Gas Analysis

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ABSTRACT: Realizing the diagnosis of lung cancer at an inchoate stage is significant to get valuable time to conduct curative surgery. In this work, we relied on a density functional theory (DFT)-proposed Ru−SnS₂ monolayer as a novel, promising biosensor for lung cancer diagnosis through exhaled gas analysis. The results indicated that the Ru−SnS₂ monolayer has admirable adsorption performance for three typical volatile organic compounds (VOCs) of lung cancer patients, which therefore results in a remarkable change in the electronic behavior of the Ru-doped surface. As a consequence, the conductivity of the Ru−SnS₂ monolayer increases after gas adsorption based on frontier molecular orbital theory. This provides the possibility to explore the Ru−SnS₂ monolayer as a biosensor for lung cancer diagnosis at an early stage. In addition, the desorption behavior of three VOCs from the Ru−SnS₂ surface is studied as well. Our calculations aim at proposing novel sensing nanomaterials for experimentalists to facilitate the progress in lung cancer prognosis.

1. INTRODUCTION
As one of the commonest cancers in our human, lung cancer has received great attention in recent years given its high incidence and mortality rates.1,2 At present, bold proteomic patterns, nuclear magnetic resonance, and chest tomography are widely applied technologies for the diagnosis of lung cancer.3,4 However, these methods are somewhat time-consuming, expensive, or invasive and what is worse is that lung cancer in most cases can only be diagnosed at an advanced stage. In other words, these so-called progressive methods cannot effectively increase the survival rate of lung cancer.

To realize the diagnosis of lung cancer at an early stage, exhaled breath analysis, based on analyzing the exhaled gas of a possible patient daily, is proposed aiming at improving the whole survival.5,6 As reported, human exhaled gas contains more than 200 volatile organic compounds (VOCs), which can reflect the potential dysfunction of human organs.7,8 VOCs that are recognized as lung cancer biomarkers are hydrocarbons such as isoprene (C₅H₈) and methyl cyclopentane (C₆H₁₂), hydrocarbon derivatives such as 1-propanol (C₃H₈O) and 2-propenal (C₃H₄O) as well as aromatic hydrocarbons such as benzene (C₆H₆) and styrene (C₈H₈).3,9 That is, if the existence of these typical gases can be detected, the subjects are possible victims of lung cancer. To this end, surface-enhanced Raman spectroscopy was reported as a good candidate for the detection of VOCs. Apart from that, chemical resistance-type sensors with high sensitivity and rapid response10−12 could also be a prospective method for the diagnosis of lung cancer through exhaled breath analysis. The sensing mechanism of such a sensor is based on the change in the conductivity of the sensing material after interaction with targeted gases.13 During the gas interaction, electrons will transfer between the adsorbent surface and gas molecules, changing the carrier concentration of the sensor and therefore modifying its electronic behavior.14 In fact, some scholars have proposed the application of resistivity-type sensors as promising devices in this field as it definitely provides a quite easy manner for the early diagnosis of lung cancer without pain and invasion.5,15 From this aspect, the materials with desirable chemical reactivity and high carrier mobility would be on priority to be exploited as potential sensors for VOCs.

Transition-metal dichalcogenides (TMDs) very recently become the focus of attention for sensing applications due to their strong chemical reactivity and high carrier mobility, especially when they are in two-dimensional (2D) structures. Among them, monolayer MoX₂ (X = S, Se, and Te) are first explored and reported to have strong potential for gas sensing...
However, a SnS$_2$ monolayer that has a similar structure and property to those of a MoS$_2$ monolayer faces a lack of attention. In fact, the SnS$_2$ monolayer has an admirable indirect semiconducting property with a band gap of 2.60 eV and a superior carrier mobility of 50 cm$^2$·V$^{-1}$·s$^{-1}$, which confers its application for gas sensors, lithium-ion batteries, and water splitting. Moreover, through n-doping or p-doping of the SnS$_2$ monolayer, much more desirable properties could be obtained. Ma et al. reported a Pd-doped SnS$_2$ monolayer for gas sensing in transformer oil, which reveals the good performance of a transition-metal-doped SnS$_2$ monolayer as a gas sensor. Moreover, it also stimulates us to utilize a Ru-doped SnS$_2$ (Ru–SnS$_2$) monolayer for VOC sensing to exploit its potential in lung cancer diagnosis. The Ru dopant has been demonstrated with good catalytic behavior for gas interaction and we believe that it can bring expected performance in VOC sensing. All of the reported results, including the optimization of the Ru–SnS$_2$ monolayer and the adsorption process, were obtained using the density functional theory (DFT) method. Our theoretical calculations can provide the sensing mechanism of the Ru–SnS$_2$ monolayer, and with the successful synthesis of large-scale atomic-layer SnS$_2$, we are hopeful that the Ru–SnS$_2$ monolayer could be explored as a novel chemical gas sensor in many fields.

2. RESULTS AND DISCUSSION

2.1. Ru Doping Behavior on the SnS$_2$ Monolayer. We defined the adsorption of one Ru dopant on the pristine SnS$_2$ monolayer to form a Ru–SnS$_2$ counterpart. The parameter of binding energy ($E_b$) was used to evaluate the chemical stability of the Ru–SnS$_2$ monolayer, the $E_b$ is calculated by the energy of Ru–SnS$_2$ subtracting the total energies of pristine SnS$_2$ and the Ru atom. Three doping sites were considered, namely, T$_{S1}$ (on top of the S atom of the first layer), T$_{Sn}$ (on top of the Sn atom of the second layer), and T$_{S2}$ (on top of the S atom of the second layer). After full optimization, the most stable configuration for Ru doping is through the T$_{S1}$ site, which possesses lower $E_b$ compared with that of the T$_{Sn}$ site. Interestingly, after the optimization of Ru doping on the T$_{S2}$ site, the Ru dopant experiences somewhat displacement, making the structure the same as that of the T$_{S1}$ site. Figure 1 plots the geometric structure and electron deformation density (EDD) of the identified Ru–SnS$_2$ monolayer.

As shown in Figure 1a, the $E_b$ of the Ru–SnS$_2$ monolayer through the T$_{S1}$ site is $-3.98$ eV, much higher than the cohesive energy of the Ru atom (0.85 eV). Moreover, it is also larger than the $E_b$ in the T$_{Sn}$ site of 3.64 eV and in the T$_{S2}$ site of 2.85 eV. These findings mean that Ru doping on the SnS$_2$ monolayer through the T$_{S1}$ site is quite thermodynamically favorable. After doping, the Ru adatom is captured by the surrounding S atoms, forming Ru–S bonds accordingly with a uniform bond length of 2.24 Å, slightly shorter than the sum of covalent radii of Ru and S atoms. This finding manifests the strong binding force in the Ru–S bond with high chemical stability. In Figure 1b, one can see that the Ru dopant is surrounded by electron depletion, indicating its electron-donating behavior, in agreement with the Hirshfeld analysis that indicates that 0.223e transfers from the Ru dopant to the SnS$_2$ monolayer. On the other hand, the electron accumulation is mainly localized on the SnS$_2$ monolayer and the Ru–S bonds, suggesting the strong electron hybridization between the Ru dopant and S atoms.

To further confirm the chemical stability of a single Ru atom on the SnS$_2$ monolayer, the diffusion of the Ru atom from the T$_{S1}$ site to the T$_{S2}$ site is investigated. As shown in Figure 2, the energy barrier for Ru diffusion is as large as 4.11 eV, much higher than that of the critical barrier of 0.91 eV for reaction to occur energy-favorably at room temperature. Therefore, we believe that the single Ru atom could be stably adsorbed on...
the SnS$_2$ monolayer through the T$_{31}$ site with a cluster-free problem.

After confirmation of the most stable configuration of the Ru−SnS$_2$ monolayer, its electronic behavior should be analyzed. Figure 3a plots the total density of state (DOS) of the pure and Ru-doped SnS$_2$ monolayer. One can see that pure SnS$_2$ monolayer performs semiconducting property without magnetic behavior. The band gap of the pristine SnS$_2$ monolayer is calculated as 1.56 eV based on its band structure (not shown here), close to the reported one of 1.61 eV based on generalized gradient approximation (GGA) calculations, indicating the accuracy of our work. While after Ru doping, the DOS is obviously left-shifted to a lower region by about 2 eV, which suggests the strong electron-donating property of the Ru adatom, leading to the n-doping of the Ru−SnS$_2$ system. At the same time, the states of the Ru dopant contribute largely to the whole DOS of the system, in which some novel states appears within the band gap of the pure SnS$_2$ system around the Fermi level. Therefore, the conductivity of the Ru−SnS$_2$ monolayer would be significantly reduced compared with that of the pure counterpart. From Figure 3b, it is seen that the Ru 4d orbital is highly overlapped by the S 3p, which manifests the strong orbital interaction between Ru and S atoms. These findings also explain the strong electron hybridization and binding force during the formation of the Rh−S bond.

Figure 4 exhibits the optimized molecular structure of three typical VOCs of lung cancer. Through analysis of bond length in different molecules, it is found that the C−H bond is measured as the same, while the C==O bond is longer than that of the C−H bond and the C==C bond is shorter than the C−C bond, indicating the stronger binding force for two C atoms in the double bond format. These results match well with the previous report.  

2.2. Adsorption of VOC Molecules. First, we initiate the analysis of the C$_3$H$_4$O adsorption system, as displayed in Figure 5. We can find that the C$_3$H$_4$O molecule prefers to be parallel to the Ru−SnS$_2$ surface on the top of the Ru dopant. However, the deformation of C$_3$H$_4$O is evident after adsorption, which is no longer a plane molecule on the Ru−SnS$_2$ monolayer, implying the geometric activation of the adsorbed gas molecules. Besides, one C atom is captured by the Ru dopant, forming a new Ru−C bond measured as 2.19 Å. That is, the Ru dopant exerts strong binding force upon the C atom of C$_3$H$_4$O, which therefore leads to the large $E_{ad}$ of −1.42 eV. From the EDD, we find that electron accumulation is mainly localized on the gas molecule, while electron depletion is on the Ru−SnS$_2$ monolayer, manifesting the electron-withdrawing property of C$_3$H$_4$O that agrees with the Hirshfeld analysis ($Q_r = −0.085e$). Besides, the Ru dopant is positively charged by 0.195e after adsorption. These results mean that 0.028e of the C$_3$H$_4$O molecule are accepted from the Ru dopant, whereas 0.057e are from the SnS$_2$ surface. In other words, Ru bridges the charge transfer from the gas molecule to the SnS$_2$ layer, thereby facilitating electron redistribution in the adsorbed system. Overall, based on all of these findings, we identify the C$_3$H$_4$O adsorption on the Ru−SnS$_2$ surface as chemisorption.

As for the C$_6$H$_6$ adsorption in Figure 6, one can see that the most stable configuration is similar to that of the C$_3$H$_4$O system, in which the C$_6$H$_6$ molecule is parallel with the SnS$_2$ layer right on top of the Rh dopant. After adsorption, the C$_6$H$_6$ molecule is slightly deformed, making the molecule a little bend toward the Ru dopant. This finding manifests the strong binding force between the Ru dopant and C$_6$H$_6$ molecule, as further confirmed by the large $E_{ad}$ of −2.07 eV. Based on the Hirshfeld method, the Ru is positively charged by 0.218e and the C$_6$H$_6$ molecule is positively charged by 0.211e after the interaction. In other words, the Ru dopant behaves as an electron bridge, enhancing the charge transfer between the Ru−SnS$_2$ monolayer and the gas molecule, which is similar to that in the C$_3$H$_4$O system. After Ru doping, the charge transfer can be remarkably intensified due to the large electron mobility and chemical reactivity of the Ru dopant, which therefore results in larger $E_{ad}$. From the EDD, one can see that electron accumulation is mainly localized on the Ru−SnS$_2$ monolayer, while electron depletion is mainly localized on the C$_6$H$_6$ molecule, which is consistent with the Hirshfeld analysis. Apart from that, the overlap of electron accumulation and electron depletion at the area between the Ru−SnS$_2$ layer and C$_6$H$_6$ molecule manifests the electron hybridization between two interaction species, which further verifies the strong adsorption performance of the Ru−SnS$_2$ monolayer toward the C$_6$H$_6$ molecule.

When it comes to the C$_5$H$_8$ system, the most stable configuration and the related EDD are depicted in Figure 7. It could be found that C$_5$H$_8$ prefers to be adsorbed on the Ru−SnS$_2$ surface through the molecule-parallel position with a...
small slope to the plane. Rather than the little deformation of the C₆H₂ molecule after adsorption, the C₅H₈ molecule is afflicted with dramatic decomposition after being trapped by the Ru dopant with the formation of two Ru−C bonds. Originally, the five C atoms in the C₅H₈ molecule are in a same plane. However, after adsorption, the C atoms approach the Ru dopant, making the molecule bend accordingly. Specifically, the C−C and C≡C bonds becomes elongated to 1.53 and 1.41 Å on the Ru−SnS₂ surface and the newly formed Ru−C bonds are measured to be 2.15 and 2.17 Å, respectively. These results indicate not only the strong activation of C₅H₈ during adsorption but also the strong binding force between the Ru

Figure 5. Adsorption configuration of the C₃H₄O system (a) and EDD (b). In EDD, the rosy areas indicate electron accumulation and the green areas indicate electron depletion; the isosurface is set to 0.008 e/Å³.

Figure 6. Adsorption configuration of the C₆H₆ system (a) and EDD (b). In EDD, the rosy areas indicate electron accumulation and the green areas indicate electron depletion; the isosurface is set to 0.008 e/Å³.

Figure 7. Adsorption configuration of the C₅H₈ system (a) and EDD (b). In EDD, the rosy areas indicate electron accumulation and the green areas indicate electron depletion; the isosurface is set to 0.008 e/Å³.
dopant and C5H8 molecule. Combined with the calculated $E_{ad}$
of $-2.40$ eV, chemisorption nature in this system could be identified. Besides, according to the Hirshfeld analysis, the C3H4O molecule as a whole transfers 0.216e to the Ru−SnS2 surface, while the Ru dopant is positively charged by 0.047e. That is to say, the Ru dopant behaves as an electron acceptor, withdrawing 0.176e from the C5H8 molecule and only 0.040e are accepted by the SnS2 monolayer. From the EDD, one can observe that electron accumulation is mainly around the Ru center and electron depletion is mainly located on the C5H8 molecule. Considering the large charge transfer between the C5H8 molecule and Ru−SnS2 monolayer, we presume that the ionic-bonding nature dominates the formation of Ru−C bonds in this system, as supported by the overlap of electron accumulation and electron depletion on the Ru−C bonds, which indicates electron hybridization during their formation.

In short, the Ru−SnS2 monolayer possesses the strongest interaction with the C3H4O molecule, followed by the C5H8 molecule and the last being the C6H6 molecule. Besides, strong chemisorption is determined in three systems. At the same time, the electron hybridization is mainly around the Ru center and electron depletion is mainly located on the C5H8 molecule. Considering the large charge transfer between the C3H4O molecule and Ru−SnS2 monolayer, we assume that the ionic-bonding nature dominates the formation of Ru−C bonds in this system, as supported by the overlap of electron accumulation and electron depletion on the Ru−C bonds, which indicates electron hybridization during their formation.

2.3. DOS of the Ru−SnS2 Monolayer upon Gas Adsorption. Figure 8 exhibits the total DOS and molecular DOS before and after gas adsorption, as well as the atomic DOS of bonding atoms to comprehensively understand the electronic behavior of the Ru−SnS2 monolayer for gas adsorption. It is seen from the total DOS that after adsorption the states of the Ru−SnS2 monolayer undergoes a different level of deformation, which is attributed to the DOS states of the adsorbed gas molecules whose states are activated to some extent. Specifically, one can see that the DOS peaks of three isolated gases split into several small peaks near the Fermi level. In that case, the electronic behavior of the gas adsorbed systems would be remarkably impacted because of the contribution of the adsorbed gas molecules around the Fermi level. On the other hand, although there are some states located at the deep valence band, we assume that they have little effect on the electronic behavior of the whole system due to their weak activation.

Moreover, from the atomic DOS of Ru and C atoms, it is found that the Ru 4d orbital is highly overlapped by the C 2p orbital, ranging from $-5$ to 3 eV for the C3H4O system and from $-5$ to 2.5 eV for C5H8 and C6H6 systems. These findings illustrate the strong electron hybridization and binding force of the Rh−C bond; this is in agreement with the previous EDD analysis. It is worth noting that the significant changes in the electronic behavior of the Ru−SnS2 monolayer will accordingly change its electrical conductivity after adsorption. Based on this evidence, the sensing mechanism of a resistance-type sensor for detecting typical gases of lung cancer could be explored.

2.4. Frontier Molecular Orbital Theory Analysis. To explore the possibility of the Ru−SnS2 monolayer as a resistance-type gas sensor for detecting typical gases of lung cancer, we, in this section, emphasize the analysis of frontier molecular orbitals to give an insight into the potential sensing mechanism of such a chemical gas sensor. Frontier molecular orbitals include highest molecular occupied orbital (HOMO) and lowest molecular unoccupied orbital (LUMO). It is well...
known that the energy gap ($E_g$) between HOMO and LUMO is an effective parameter to evaluate the electrical conductivity of certain surfaces. Specifically, large $E_g$ reveals small electrical conductivity and small $E_g$ reveals large electrical conductivity.

Figure 9 exhibits the HOMO and LUMO distributions, their related energies, and the calculated $E_g$ in various systems. It could be seen in the isolated Ru−SnS$_2$ system that HOMO and LUMO are all mainly located at the Ru dopant, while there also exist some HOMOs and LUMOs on the SnS$_2$ surface.

Besides, the energies of HOMO and LUMO for the Ru−SnS$_2$ monolayer are calculated to be −5.87 eV and −4.96 eV, respectively, and therefore, the $E_g$ is 0.91 eV. This finding indicates its semiconducting behavior and manifests its suitability for gas sensing applications.

When it comes to the gas adsorbed systems, one can see that the HOMO and LUMO distributions of the Ru−SnS$_2$ monolayer experience pronounced changes. In the C$_3$H$_4$O system, one can see that HOMO is mainly around the Ru dopant and LUMO is localized on the SnS$_2$ layer, while there only has a few HOMOs and LUMOs on the C$_3$H$_4$O molecule; in the C$_6$H$_6$ system, the HOMO is mainly on the Ru dopant and in the area between the Ru adatom and C$_6$H$_6$ molecule, whereas the LUMO is largely localized on the Ru dopant; in the C$_5$H$_8$ system, the HOMO and LUMO are both mainly localized on the Ru dopant and a few are on the gas molecule.

Along with these, changes in their distribution are the related changes in their energies and subsequently their $E_g$ that finally determine the electrical conductivity of the system. Detailedly, the $E_g$ in the C$_3$H$_4$O system declines to 0.29 eV; in the C$_6$H$_6$ system, it declines to 0.53 eV; and in the C$_5$H$_8$ system, it declines to 0.30 eV. As mentioned, the reduced $E_g$ would result in an increase in conductivity of the Ru−SnS$_2$ monolayer after the adsorption of three typical gases. Moreover, the significant change in $E_g$ will lead to evident changes in electrical conductivity. In this regard, we assume that the Ru−SnS$_2$ monolayer is a promising candidate for C$_3$H$_4$O, C$_6$H$_6$, and C$_5$H$_8$ sensing given the admirable change in its $E_g$ after their adsorption. Moreover, for exhale gas analysis, using a Ru−SnS$_2$-based gas sensor can realize an effective detection and as a result make an accurate diagnosis for possible lung cancer.

### 2.5. Recovery Property
To further characterize the possible use of the Ru−SnS$_2$ monolayer as a chemical sensor for lung cancer diagnosis, the recovery property is analyzed to determine the reusability of the typical sensor. The recovery behavior is the required minimum time for a sensor to desorb the adsorbed gases from its surface, in which the recovery time ($\tau$) is explained by the transition state theory and the van’t Hoff−Arrhenius expression

$$\tau = A^{-1} e^{(-E_a/k_BT)}$$

where $A$ is the attempt frequency defined as $10^{12}$ s$^{-1}$, $k_B$ is the Boltzmann constant ($8.318 \times 10^{-3}$ kJ/(mol·K)). Also, the $E_a$ (potential barrier) of desorption is equal to the value of $E_{ad}$ due to the inverse process between the adsorption and desorption. It could be deduced that a larger $E_{ad}$ would increase the difficulty for gas desorption and a temperature increase can accelerate that process largely. Based on our calculated $E_{ad}$ in this work, however, the recovery time for such three typical gases of lung cancer from Ru−SnS$_2$ surface would be too long and even unrealistic at room temperature. On the other hand, when the temperature is higher than 600 K, the desorption becomes possible in one day. Considering the heat loss and the sanitary safety of the devices, we recommend the one-off operation of the gas sensors for the diagnosis of lung cancer. From this aspect, it is hopeful that Ru−SnS$_2$-based gas sensors with high sensitivity for typical gases of lung cancer could be further explored in the laboratory to extend their applications in the field of clinical medicine.

### 3. CONCLUSIONS
Using DFT, we theoretically investigated the Ru doping behavior on the SnS$_2$ monolayer and simulated the adsorption behavior of Ru−SnS$_2$ for three typical gases of lung cancer to explore its potential as a resistance-type sensor for lung cancer diagnosis. The main conclusions are as follows:

(i) A single Ru atom could be stably doped on the SnS$_2$ monolayer with high chemical stability and strong binding force without a cluster problem.

(ii) The Ru−SnS$_2$ monolayer possesses high chemisorption of three gasses that brings a significant change in its electronic property.
(iii) After adsorption of typical gases of lung cancer, the conductivity of the Ru–SnS₂ monolayer could be increased, which provides the possibility for its exploration as biosensors for the diagnosis of lung cancer at an early stage.

Based on these, we suggest to explore Ru–SnS₂ as a resistance-type gas sensor in the clinical medicine. We are hopeful that our calculation could provide some guidance for its further exploration in other fields as well.

4. COMPUTATIONAL DETAILS

The DFT calculations were completed in the D mol³ package in a spin-polarized manner. To deal with the electron exchange–correlation terms, the Perdew–Burke–Ernzerhof (PBE) function with generalized gradient approximation (GGA) was considered. The DFT-D2 method was adopted to understand the Van der Waals force and long-range interactions, as proposed by Grimme. Double numerical plus polarization (DNP) was selected as the atomic orbital basis set, and the energy tolerance accuracy, maximum force, and displacement were determined as 10⁻³ Ha, 2 × 10⁻³ Ha/Å, and 5 × 10⁻³ Å, respectively. The Brillouin zone Monkhorst-Pack grid was sampled with a k-point mesh of 5 × 5 × 1 for the supercell geometric optimizations and of 10 × 10 × 1 for related electronic calculations. For static electronic structure calculations, a self-consistent loop energy of 10⁻⁴ Ha was determined to ensure the accurate results of the total energy.

A 3 × 3 supercell containing 16 Sn atoms and 18 S atoms was established as the SnS₂ monolayer, on which one Ru atom was adsorbed to form the Ru–SnS₂ monolayer. The constant parameters of the pristine and Ru-doped SnS₂ monolayer were both calculated as 3.7 Å, in line with the previous report. For gas adsorption, the vacuum layer of 15 Å was used to prevent the interaction between adjacent units. The adsorption energy \( E_{\text{ad}} \) is introduced to evaluate the interaction strength of adsorbing processes, calculated by the formula

\[
E_{\text{ad}} = E_{\text{surf/gas}} - E_{\text{surf}} - E_{\text{gas}}.
\]

In this formula, \( E_{\text{surf/gas}}, E_{\text{surf}}, \) and \( E_{\text{gas}} \) represent the energies of the gas adsorbed system, the pure Ru–SnS₂ surface, and pure gas species, respectively. In the meanwhile, Hirshfeld analysis was considered for charge transfer \( (Q_{\text{T}}) \) during gas adsorptions. The positive \( Q_{\text{T}} \) means the electron-donating behavior of the adsorbed gas molecule, while the negative \( Q_{\text{T}} \) indicates the electron-accepting behavior of the adsorbed gas molecule.

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Notes
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