

Article

Ru-Doped PtTe₂ Monolayer as a Promising Exhaled Breath Sensor for Early Diagnosis of Lung Cancer: A First-Principles Study

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Abstract: Using the first-principles theory, the geometric and electronic properties of the Ru-doped PtTe₂ (Ru-PtTe₂) monolayer, and its sensing performance for three VOCs biomarkers, namely, 2-propenal (C₃H₄O), acetone (C₃H₆O) and isoprene (C₅H₈), were analyzed, to expound its potential for exhaled breath analysis and diagnosis of lung cancer. It was found that the Ru-substitution on the surface of the pristine PtTe₂ surface with a Te atom is energy-favorable, with the formation energy of −1.22 eV. Upon adsorption of the three VOC gas species, chemisorption was identified with the adsorption energies of −1.72, −1.12 and −1.80 eV for C₃H₄O, C₃H₆O and C₅H₈, respectively. The Ru-doping results in a strong magnetic property for the PtTe₂ monolayer, whereas the gas adsorption eliminates this magnetic behavior. The electronic properties reveal the sensing mechanism of the Ru-PtTe₂ monolayer for gas detection, and the bandgap change indicates its admirable positive sensing response for the three gas species. Therefore, we conclude that the Ru-PtTe₂ monolayer is a promising sensing material to realize the diagnosis of lung cancer through exhaled gas detection, with a remarkable decrease in its electrical conductivity. This work paves the way for further exploration of the PtTe₂-based gas sensor for early diagnosis of lung cancer, and we hope that more sensing materials can be investigated using the PtTe₂ monolayer.

Keywords: ru-PtTe₂; exhaled breath analysis; gas sensor; first-principles theory; lung cancer



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1. Introduction

Lung cancer, the second most prevalent cancer, has the highest morbidity and mortality rates among adult people [1], posing a great threat to human health globally. However, the current technologies used to make a definite diagnosis of lung cancer, including bold proteomic patterns, nuclear magnetic resonance and chest tomography [2,3], are at an advanced stage, and thus provide no significant benefits to increase the survival rate for a lung cancer patient. Therefore, the early diagnosis of lung cancer is essential to increasing such prospects. It is reported that growing tumors in the human body can release several volatile organic compounds (VOCs) into the blood, which can then be exchanged in the lung [4]. Therefore, the exhaled VOCs of a lung cancer patient are remarkably higher in comparison with those of a healthy person [5]. Scholars in this field have thus proposed exhaled breath analysis to identify possible patients and related severity [6–8]. This has been regarded as a rapid and workable approach, which does not cause trauma, to address the issue of lung cancer [9,10]. Such VOCs, including hydrocarbons such as isoprene (C₅H₈), hydrocarbon derivatives such as acetone (C₃H₆O) and 2-propenal (C₃H₄O), and several aromatic hydrocarbons [11–13], are so-called biomarkers that show the dysfunction severity of human lungs. Given the low concentration of the biomarkers of lung cancer, which are within the ppm level, the gas-sensing technique should have the advantage of high sensitivity to gas species.

Regarding VOC detection, the nanosensing method has great potential, with the advantages of low cost, high sensitivity and rapid response [14,15]. In recent years, the

transition-metal dichalcogenides (TMDs), discovered as novel two-dimension (2D) materials with a tunable semiconducting property [16–18], have been closely studied as novel sensing materials for gas detection [19–21]. Increasingly, the noble TMDs, such as PtS₂ and PtSe₂, have been theoretically and experimentally proven to have diverse electronic properties in comparison with the popular TMDs such as MoS₂ and MoSe₂ [22–24]. Specifically, PtS₂ and PtSe₂ monolayers have been demonstrated to have a high sensing response and short response time [25,26], and thus have high potential as gas sensors. In addition, metal-doping can significantly promote the adsorption and sensing behaviors of the sensing material for gas species [27–29], which allows their typical application in harsh environments, with good sensitivity [30]. By comparison, the PtTe₂ monolayer and its TM-doped counterparts, to the best of our knowledge, have been less explored for gas sensing applications, although the geometric and electronic properties of TM-doping are well-predicted in previous studies [31–33]. In this regard, the TM-doped PtTe₂ monolayer may be a promising candidate with admirable sensing performance for gas detection, which stimulated the focus of our attention on this field [34,35].

In this work, we simulated the adsorption and sensing performance of a Ru-doped PtTe₂ (Ru-PtTe₂) monolayer for three typical VOCs, namely, C₃H₄O, C₃H₆O and C₅H₈, to investigate its potential as a gas sensor for lung cancer diagnosis. The Ru atom, which has been proven to have good catalytic behavior for gas interactions [36–38], was selected and replaced with a Te atom of the PtTe₂ monolayer to establish the Ru-PtTe₂ structure, and we believed that this may result in favorable performance for VOC sensing. The adsorption of three VOC molecules on the Ru-PtTe₂ monolayer without considering the existence of oxygen or humidity was conducted in order to directly analyze the adsorption and sensing mechanism of the Ru-doped surface, so as to explore its theoretical potential as a gas sensor. All the simulations were theoretical calculations based on the first-principles theory, which can provide a comprehensive understanding of the Ru-PtTe₂ surface and the gas molecule. However, the gas concentration in the current work could not be considered. Through this work, in the future, we aim to uncover the gas-sensing mechanism of the Ru-PtTe₂ monolayer for VOCs, and hope to facilitate further cutting-edge investigations, especially in terms of experimental insights into PtTe₂-based gas sensors.

2. Computational Methods

We carried out all of the first-principles simulations in the DMol³ package [39], and selected the generalized gradient-approximation (GGA) within the Perdew Burke Ernzerhof (PBE) function to determine the electron correlations and exchange [40]. A *k*-point mesh of 10 × 10 × 1 was sampled for geometric optimizations and the electronic calculations [41]. The Van der Waals force and the long-term reaction were treated by the dispersion-corrected DFT-D2 method, as proposed by Tkatchenko and Scheffler [42]. The energy tolerance accuracy and the global orbital cut-off radius were defined as 10^{−5} Ha and 5.0 Å, respectively, to ensure good accuracy of the calculated total energies for the structures [43].

A 4 × 4 × 1 supercell was established for the PtTe₂ monolayer, which includes 18 Te atoms and 9 Pt atoms, to carry out the simulations, and a 20 Å vacuum area along the *z* direction to eliminate the interface interactions [44]. Furthermore, the Hirshfeld method was used to analyze the charge transfer (*Q_T*) in the gas adsorption systems, by which the negative values indicated the electron-accepting property of the gas molecules. The charged value of the Ru dopant (*Q_{Ru}*) was analyzed in the same way. Moreover, the adsorption processes were conducted at room temperature, to obtain the optimized geometric structures and related parameters.

3. Results and Discussion

3.1. Morphologies of Gas Species and Ru-PtTe₂ Monolayer

Figure 1 plots the optimized structures of three specific exhaled VOCs of lung cancer patients. One can find from the aspect of the bond length that the C-H, C-C, C=O and C=C

bonds have the same length, although in different molecules, and the C=C bond is longer than the C=O bond but is shorter than the C-C bond. These findings reveal the stronger binding force for two atoms in their double bond format, and are consistent with a previous reference [45].

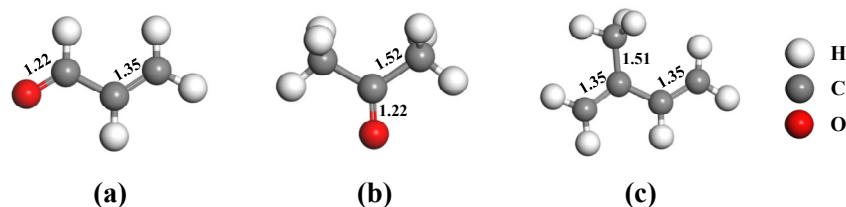


Figure 1. Morphologies of (a) C_3H_4O , (b) C_3H_6O and (c) C_5H_8 . The black values are bond length, with unit in Å.

In this work, a Te atom of the pristine $PtTe_2$ monolayer was replaced by a Ru atom to model the Ru- $PtTe_2$ monolayer, in which the Ru-doping concentration was obtained as 3.7%, which is large enough for a $4 \times 4 \times 1$ supercell, as previously mentioned [46,47]. This process is plotted in Figure 2. Moreover, the formation energy (E_f) is defined in the current work to estimate the difficulty of such process, calculated by Equation (1) [48]:

$$E_f = E_{Ru-PtTe_2} - E_{PtTe_2} - \mu_{Ru} + \mu_{Te} \quad (1)$$

where $E_{Ru-PtTe_2}$ and E_{PtTe_2} are the total energies of the Ru- $PtTe_2$ and intrinsic $PtTe_2$, respectively, and μ_{Ru} and μ_{Te} represent the chemical potential per Ru and Te atom in their bulk structures, respectively. Moreover, we repeatedly conducted the adsorption process to verify the good accuracy and repeatability of the adsorption parameters, and found that the accuracy of the current results, namely, the difference in the results among multiple simulations, can be 99.6%.

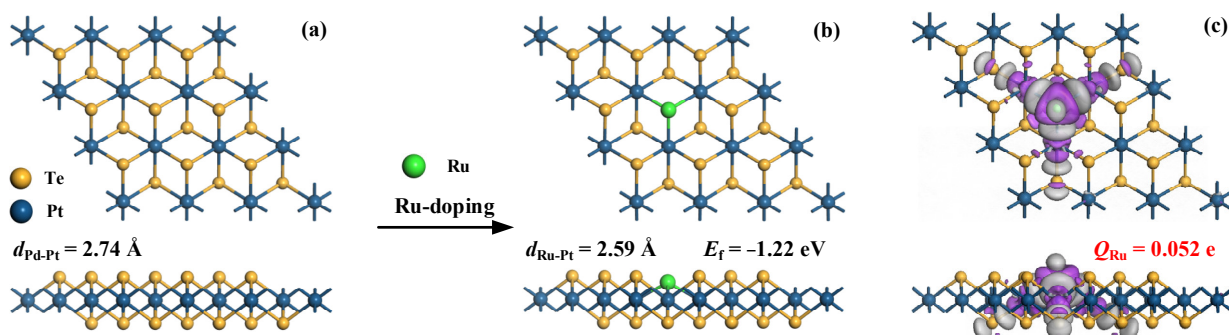


Figure 2. Ru-doping property on the $PtTe_2$ surface: (a) morphology of intrinsic $PtTe_2$ monolayer, (b,c) morphology and CDD of Ru- $PtTe_2$. In CDD, the grey and purple areas are electron accumulation and electron depletion, and the isosurface is $0.01 \text{ eV}/\text{\AA}^3$.

Figure 2a depicts the morphology of the pristine $PtTe_2$ monolayer. It can be seen that the Pt-Te bond is measured to be $2.74 \text{ \AA}$, and the length of its constant lattice, from our calculations, is $4.03 \text{ \AA}$, which are in good agreement with previous reports of 2.76 and $4.02 \text{ \AA}$, respectively [31]. The morphology of the Ru- $PtTe_2$ monolayer is shown in Figure 2b. It can be seen that the Ru dopant, on the substituted Te atom, seems to be located within the upper Te layer, making the Ru-Pt bond lengths (equally as $2.59 \text{ \AA}$) shorter than the original Pt-Te bond length ($2.74 \text{ \AA}$). This phenomenon can be ascribed to the larger atomic radii of the Te atom ($1.26 \text{ \AA}$) in comparison with the Ru dopant ($1.20 \text{ \AA}$) [49]. Based on Equation (1), the E_f for Ru-doping on the intrinsic $PtTe_2$ monolayer is increased to -1.22 eV , which means the Ru-doping process can release 1.22 eV to the surroundings of the $PtTe_2$ monolayer. In other words, the substitution of a Ru atom with a

Te atom in the pristine PtTe₂ monolayer is fully exothermic and energy-favorable, and can occur spontaneously at room temperature [50,51]. Furthermore, the vibrational analysis shows that the frequencies of the Ru-PtTe₂ monolayer range from 51.4 to 504.48 cm⁻¹; without the imaginary frequency, this indicates its good chemical stability. Therefore, the Rh-PtTe₂ monolayer can stably exist at room temperature without being affected by the volatilization issue, which allows its packaging for exploration of gas-sensing devices in the field of healthcare. From Figure 2c, in which the charge-density-difference (CDD) of the Ru-PtTe₂ monolayer is shown, it can be seen that the electron accumulations are mainly on the Ru-Pt bonds, whereas the electron depletion occurs predominantly on the Ru atom. These distributions suggest the electron hybridization on the Ru-Pt bonds, in addition to the charge-donating property of the Ru atom that releases 0.052 e to the PtTe₂ surface [28].

Figure 3 exhibits the band structure (BS) of pristine and Ru-doped PtTe₂, and the orbital density of state (DOS) of the Ru and Pt atoms, to further elucidate the electronic properties of the PtTe₂ surface caused by Ru-doping. First, focusing on the BS of the pristine PtTe₂ monolayer, one can see that the bandgap is calculated to be 0.617 eV, and the valence band maximum is located at the Γ point and the conduction band minimum is located at the K point. These suggest that the pure PtTe₂ monolayer has an indirect semiconducting property, in agreement with a previous study [52]. From the BS of the Ru-PtTe₂ monolayer, it is seen that the obtained bandgap is 0.169 eV, and the spin-up is not symmetric with the spin-down, indicating its magnetic property. This differs from the BS distribution of the pristine PtTe₂ system, wherein the spin-up overlaps with the spin-down, indicating its non-magnetic property. From our calculations, the magnetic moment of the Ru-PtTe₂ monolayer is obtained as 2.16, of which the magnetic moment of the Ru dopant is calculated as 2.04. This indicates the dominant magnetic property of the Ru dopant in this system. These findings reveal that Ru-doping results in a strong magnetic property for the PtTe₂ monolayer. In addition, the bandgap is remarkably reduced by 0.448 eV (by 72.6%), which may result from the newly generated impurity states by Ru-doping within the bandgap of the PtTe₂ system [53]. Furthermore, the valence-band maximum and conduction-band minimum are located at different points, which indicates that the Ru-doping exerts little impact on the indirect semiconducting property of the PtTe₂ monolayer. In addition, the state density in the Ru-PtTe₂ monolayer seems to be much denser compared with that of the pristine counterpart, revealing the more favorable chemical reactivity and carrier mobility of the Ru-doped system [54,55]. From the orbital DOS, it can be seen that the Ru 4*d* orbital is highly hybridized with the Pt 5*d* orbital from −5.6 to −0.5 eV and 0.3 to 1.0 eV, which implies strong orbital interactions exist between Ru and Pt atoms, agreeing with the CDD distribution in which the Ru-Pt bonds are surrounded by the electron accumulation [56]. Moreover, the asymmetric spin-up and spin-down in the Ru 4*d* orbital reveals its magnetic property in the Ru-PtTe₂ monolayer, which to some extent also leads to the slight magnetic property for the Pt atom, in which the orbital states around the Fermi level are also symmetric.

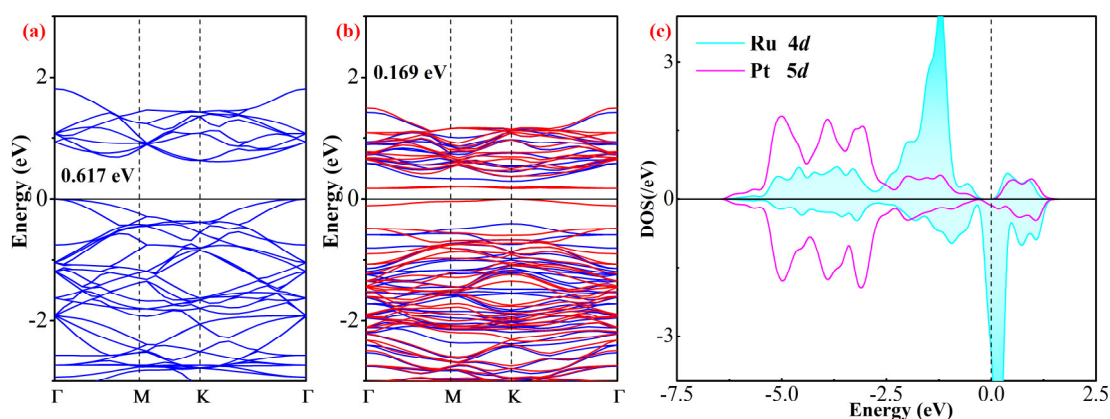


Figure 3. (a,b) BS of pristine and Ru-doped PtTe_2 systems; (c) orbital DOS of Ru and Pt atoms. In the BS, the black values are bandgaps, the black lines are spin-up, and the red lines are spin-down; in the DOS, the dash line is the Fermi level.

3.2. Adsorption VOCs on Ru-PtTe₂ Monolayer

We performed the adsorption of three VOCs on the obtained Ru-PtTe₂ monolayer, on which the gas species kept the atomic distance of appropriate 2.5 Å with the Ru dopant to implement the interactions. Moreover, the adsorption energy (E_{ad}) was employed to determine the adsorption performance of the Ru-PtTe₂ monolayer upon VOC molecules, calculated by [57]:

$$E_{\text{ad}} = E_{\text{Ru-PtTe}_2/\text{gas}} - E_{\text{Ru-PtTe}_2} - E_{\text{gas}} \quad (2)$$

where $E_{\text{Ru-PtTe}_2/\text{gas}}$ and E_{gas} signify the total energies of the Ru-PtTe₂/gas system and free gas molecule, respectively. We identified the adsorption structure with the most negative E_{ad} as the most stable configuration (MSC) and analyzed its structural and electronic properties, as presented in the following sections. The MSC and related CDD are displayed in Figure 4.

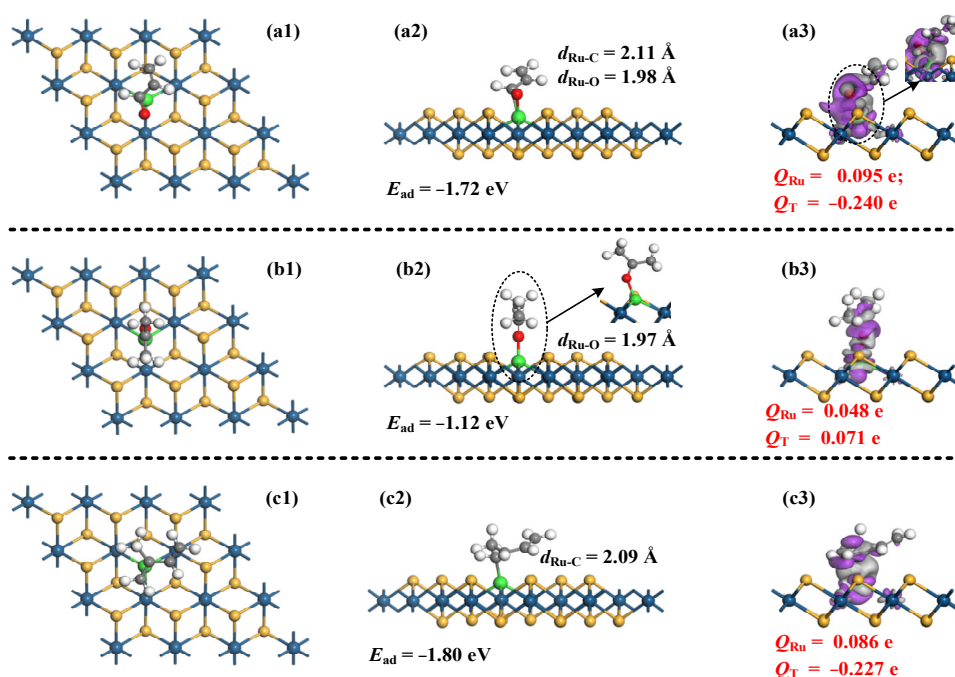


Figure 4. MSC and CDD of C₃H₄O system (a1–a3), C₃H₄O system (b1–b3) and C₅H₈ system (c1–c3). In CDD, the set is the same as in Figure 1.

In the C_3H_4O -adsorbed system, it can be seen that the C and O atoms of the $C=O$ bond in the C_3H_4O molecule are both trapped by the Ru dopant, and the formed Ru-C and Ru-O bonds are measured to be 2.11 and 1.98 Å, respectively. Three Ru-Pt bonds are measured to be 2.56, 2.59 and 2.67 Å, respectively, which indicates that the Ru atom suffers a slight displacement in C_3H_4O adsorption [47]. The E_{ad} for the C_3H_4O system is calculated to be -1.72 eV, which can be classified as chemisorption here, since its absolute value is much larger than the critical value (0.80 eV) for this identification [58]. At the same time, the C_3H_4O molecule as a whole, based on the Hirshfeld analysis, is negatively charged by 0.240 e, whereas the Ru atom is positively charged by 0.095 e. From these results, we can infer that the accepted 0.240 e of the C_3H_4O is donated by the Ru dopant (0.043 e) and the $PtTe_2$ monolayer (0.197 e), which reveals the desirable electron-donating property of the $PtTe_2$ surface and the electron-withdrawing property of the C_3H_4O molecule [59]. In the CDD distribution, it can be seen that the Ru dopant is surrounded by electron depletions, while the Ru-C and Ru-O bonds are surrounded by the electron accumulations, which confirms the electron-releasing behavior of the Ru atom and the electron hybridization on the newly formed bonds.

Upon C_3H_6O adsorption on the Ru- $PtTe_2$ monolayer, it is seen that the C_3H_6O molecule is basically vertical to the $PtTe_2$ surface, and the O atom is bonded with the Ru dopant, with the bond length measured to be 1.97 Å. Three Ru-Pt bonds are measured to be 2.55, 2.59 and 2.59 Å, respectively; the deformations are not as dramatic as those in the C_3H_4O system, indicating the weaker interaction in the C_3H_6O system. From the E_{ad} of -1.12 eV, whose absolute value is smaller than that in the C_3H_4O system, the assumption above can be verified. However, chemisorption can also be confirmed here, given its larger absolute value than the critical value [58]. Based on the Hirshfeld analysis, the C_3H_6O molecule is charged by 0.071 e and the Ru dopant is charged by 0.048 e. These findings indicate that the C_3H_6O molecule releases 0.071 e, which is separately accepted by the Ru dopant (0.004 e) and the $PtTe_2$ surface (0.067 e). These phenomena are also different from those of the C_3H_4O system, in which the C_3H_6O has an electron-releasing property and the Ru- $PtTe_2$ monolayer behaves as an electron acceptor. From the CDD, the electron depletion is mainly on the C_3H_6O molecule and the electron accumulation is mainly on the Ru-O bond, which confirms the above analysis of the electron-releasing property of the C_3H_6O , and the strong binding force between the Ru dopant and the O atom.

Regarding the C_5H_8 system, it can be seen that the C atom of the C-C bond in the C_5H_8 molecule, instead of the $C=C$ bond, is trapped by the Ru dopant, with the formed Ru-C bond measured as 2.09 Å. Three Ru-Pt bonds are measured as 2.56, 2.63 and 2.67 Å, respectively. These values indicate that the Ru dopant suffers the largest deformations among the three systems, implying the strongest molecular interaction here, as verified by the E_{ad} (-1.80 eV), which indicates the C_5H_8 system has the strongest chemisorption among the three VOC-adsorbed systems. The Hirshfeld analysis reveals that the C_5H_8 molecule accepts 0.227 e from the Ru- $PtTe_2$ monolayer, in which the Ru atom donates 0.034 e while the $PtTe_2$ surface donates 0.193 e. This phenomenon is similar to that in the C_3H_4O system, in which the gas species has a strong electron-accepting property, whereas the Ru- $PtTe_2$ monolayer has a strong electron-donating property. From the CDD, it can be seen that the C_5H_8 molecule and the Ru-C bond are mainly surrounded by the electron accumulations, which supports the above analysis.

In summary, chemisorption was identified for all three Ru- $PtTe_2$ VOC-adsorbed systems, and the adsorption strength had the order of $C_5H_8 > C_3H_4O > C_3H_6O$. Given the desirable adsorption performance, to some extent the electronic and magnetic properties may also be impacted, which is analyzed in detail in the next section.

3.3. Electronic Properties of the Gas Systems

The electronic properties of the Ru- $PtTe_2$ monolayer upon VOC adsorption were analyzed by the BS and orbital DOS, as exhibited in Figure 5. From the BS of C_3H_4O , C_3H_6O and C_5H_8 systems, it can be seen that the bandgaps of these three systems are

calculated as 0.540, 0.618 and 0.654 eV, respectively. These reveal the dramatic deformations of the electronic property in the Ru-PtTe₂ monolayer caused by VOC adsorptions, which can also bring about a remarkable change in the electrical conductivity of the Ru-PtTe₂ monolayer. In addition, the spin-up is symmetrical with the spin-down in the three gas-adsorbed systems, which indicates the non-magnetic property of the Ru-PtTe₂/gas systems, as verified by the calculated magnetic moment of 0 in three systems. In other words, the VOC gas adsorptions eliminate the magnetic property of the isolated Ru-PtTe₂ monolayer.

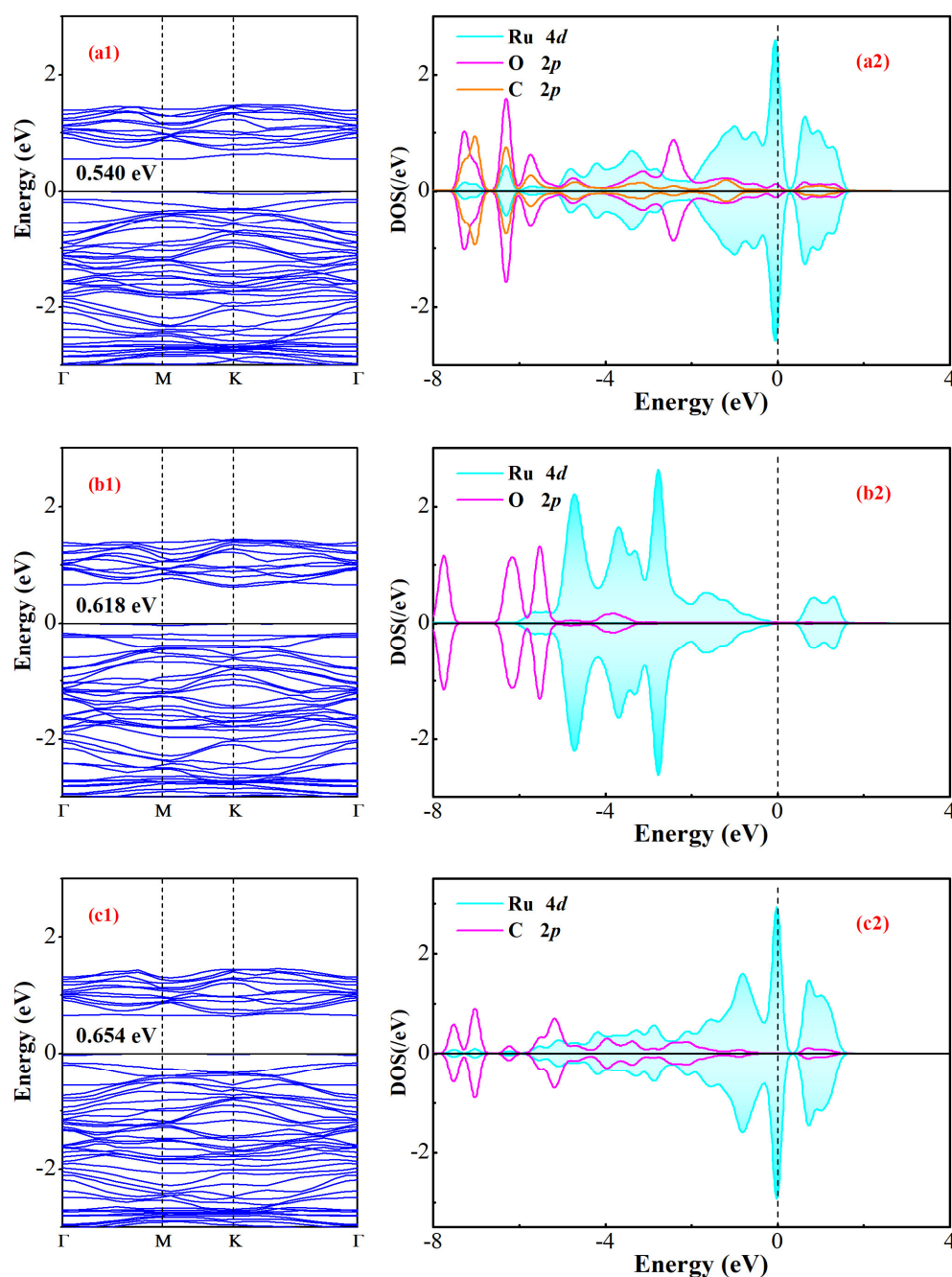


Figure 5. BS and orbital DOS of (a1,a2) C₃H₄O, (b1,b2) C₃H₆O and (c1,c2) C₅H₈ systems.

From the orbital DOS of bonded atoms in the three systems, it can be seen that the states of the Ru 4d orbital are highly overlapped with the bonded O and C 2p orbitals of C₃H₄O, the O 2p orbital of C₃H₆O, and the C 2p orbital of C₅H₈. Specifically, the overlaps are located at −7.3, −7.0, −6.3, −5.8, −4.8 to −0.1, and 0.6 to 1.3 eV in the C₃H₄O system;

at -5.5 , -3.8 and 0.7 eV in the C_3H_6O system; and at -7.5 , -7.0 , -6.2 , -5.6 to -0.9 and 0.6 to 1.3 eV in the C_5H_8 system. These orbital hybridizations reveal the strong orbital interactions between the Ru dopant and the bonded atoms, which facilitate their formations but also verify the strong binding force in the VOC adsorption systems that leads to the chemisorption. Moreover, it is these strong orbital interactions that modulate the electronic property of the Ru-PtTe₂ monolayer in the gas adsorptions, which gives rise to the possible detection of these gas species through the change in electronic property.

3.4. Gas Sensing Explorations

The change in the electronic property in the Ru-PtTe₂ monolayer in the VOC-adsorbed systems provides strong potential for its exploration as a resistance-type gas sensor. As mentioned in the bandgap results, the bandgap increased by 0.540 eV in the C_3H_4O system, by 0.449 eV in the C_3H_6O system, and by 0.485 eV in the C_5H_8 system. According to the relationship between the bandgap (B_g) and the electrical conductivity (σ), as illustrated in Equation (3), it can be inferred that the electrical conductivity of the Ru-PtTe₂ monolayer would be reduced most significantly after C_5H_8 adsorption, followed by the adsorption of C_3H_6O , and, finally, the adsorption of C_3H_4O .

$$\sigma = \lambda \cdot e^{(-B_g/2kT)} \quad (3)$$

where λ is the constant, k is the Boltzmann constant (8.318×10^{-3} kJ/(mol·K)) and T is temperature. In other words, the sensing response in these three systems can be ranked as $C_5H_8 > C_3H_6O > C_3H_4O$. Moreover, the sensing response (S), related to the electrical resistance of the nano-sensing material, can be formulated as [60]:

$$S = (\sigma_{\text{gas}}^{-1} - \sigma_{\text{pure}}^{-1}) / \sigma_{\text{pure}}^{-1} \quad (4)$$

in which σ_{gas} and σ_{pure} are, separately, the electrical conductivity of the Ru-PtTe₂/gas system and isolated Ru-PtTe₂ system. According to these two formulas, we can calculate that the sensing response (S) for sensing C_5H_8 , C_3H_6O and C_3H_4O are 1.37×10^3 , 6.26×10^3 and 1.26×10^4 , respectively, at room temperature (298 K). In this regard, we can conclude that the Ru-PtTe₂ monolayer has positive sensitivity for the three VOC gas species [61], and the sensing response of the Ru-PtTe₂/gas systems in a real experiment are large enough to realize sensitive detection, given the good sensing property within the determined crystal, based on certain electrochemical workstations that enable resistance measurement [62,63]. That is, the Ru-PtTe₂ monolayer is an outstanding VOC sensor for conducting C_5H_8 , C_3H_6O and C_3H_4O sensing with desirable sensitivity.

In addition, it is well known that the existence of oxygen (O_2) and humidity (H_2O) can exert a dramatic impact on the gas adsorption and sensing properties of nanomaterials. To comprehend their effects in this work, we performed the co-adsorption of VOCs and O_2 (or H_2O) molecules and analyzed their BS configurations, with the results depicted in Figure 6. From this figure, one can see that the existence of the O_2 molecule weakened the adsorption performance, whereas the existence of the H_2O molecule largely enhanced the adsorption performance of the Ru-PtTe₂ monolayer for the three VOCs, from the calculated values of E_{ad} . However, it should be mentioned that, in the three systems having O_2 , the bandgaps are largely reduced, especially for the C_3H_6O system, in which there are several novel states crossing the Fermi level, giving the system a metallic property with a bandgap of 0.000 eV [64]. In other words, the existence of the O_2 molecule can cause strong n-type doping for the VOC-adsorbed systems, therefore dramatically reducing the electrical conductivity of the Ru-PtTe₂ monolayer, which is quite beneficial to promoting the sensing responses for gas detection [65]. Furthermore, along with the enhanced adsorption performance of the Ru-PtTe₂ monolayer in the three systems having H_2O , the bandgaps are also slightly reduced, which also promotes the electrical conductivity of the Ru-PtTe₂ monolayer for VOC sensing in the presence of H_2O to some extent. From all of the analyses above, one can presume that a Ru-PtTe₂-based device is a promising candidate for diagnosing lung cancer by a

tester using the sensing mechanism of the reduced electrical resistance of exhaled breath, especially in an atmosphere including oxygen and humidity.

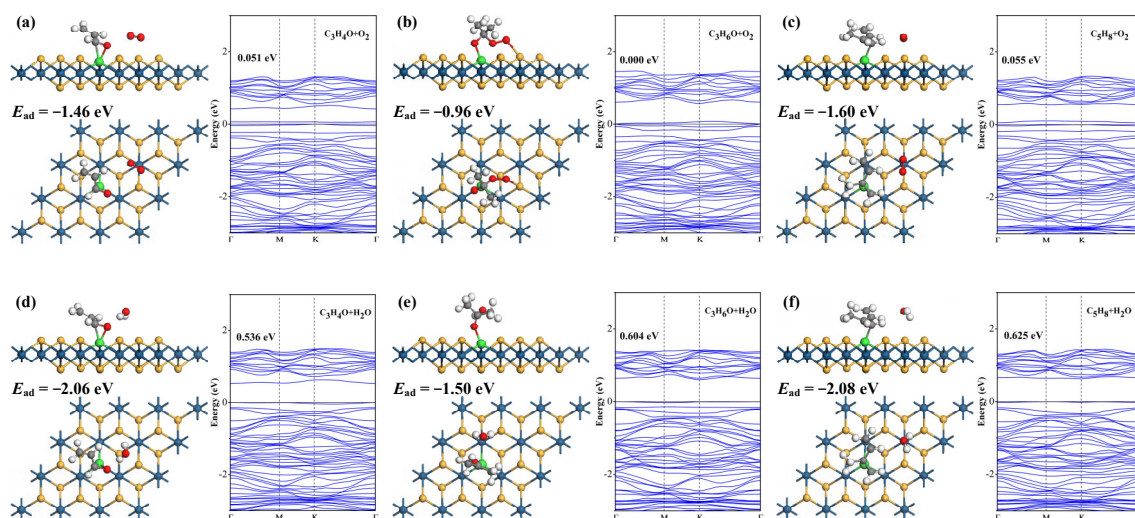


Figure 6. Gases' co-adsorption configurations and BS of O_2 (or H_2O) and VOCs: (a) C_3H_4O/O_2 system, (b) C_3H_6O/O_2 system, (c) C_5H_8/O_2 system, (d) C_3H_4O/H_2O system, (e) C_3H_6O/H_2O system and (f) C_5H_8/H_2O system.

4. Conclusions

In this work, we propose the Ru-PtTe₂ monolayer as a promising sensing candidate for three typical VOCs, in order to perform exhaled breath analysis for a potential lung cancer patient. The main conclusions are as follows:

- the Ru-doping process on the pristine PtTe₂ monolayer by Te-substitution is fully energy-favorable, with E_f of -1.22 eV;
- the Ru-PtTe₂ monolayer performs chemisorption on the three VOC gas species, and E_{ad} is obtained as -1.72 , -1.12 and -1.80 eV for C_3H_4O , C_3H_6O and C_5H_8 , respectively;
- Ru-doping results in a strong magnetic property for the PtTe₂ monolayer, whereas the gas adsorption eliminates this magnetic behavior;
- the change in the bandgap in the Ru-PtTe₂ monolayer indicates its admirable sensing response for the three gas species, obtained as 1.37×10^3 , 6.26×10^3 and 1.26×10^4 in C_3H_4O , C_3H_6O and C_5H_8 systems, respectively.

In summary, the Ru-PtTe₂ monolayer is a promising sensing material for the detection of biomarkers in exhaled breath, and provides the potential to identify lung cancer through exhaled gas detection with a good sensing response.

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