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Sn$_3$C$_2$ monolayer with transition metal adatom for gas sensing: a density functional theory studies

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Abstract
The gas sensing properties of pristine Sn$_3$C$_2$ monolayer and different transition metal adatom (TM-Sn$_3$C$_2$, where TM = Fe, Co, Ni, Cu, Ru, Rh, Pd and Ag) was investigated using van der Waals corrected density functional theory. The understanding and potential of use of Sn$_3$C$_2$ monolayers as sensors or adsorbent for CO, CO$_2$, NO, NO$_2$ and SO$_2$ gaseous molecules is evaluated by calculating the adsorption and desorption energetics. From the calculated adsorption energies, we found that the pristine Sn$_3$C$_2$ monolayer and 3$d$ TM has desirable properties for removal of the considered molecules based on their high adsorption energy, however the 4$d$ TM is applicable as recoverable sensors. We applied an Arrhenius-type equation to evaluate the recovery time for the desorption of the molecules on the pristine and TM adatom on Sn$_3$C$_2$ monolayer. We found that the negative adsorption energies from $-1$ to $-2$ eV of the molecules resulted in easier recovery of the adsorbed gases at reasonable temperatures compared to adsorption energies in between 0 and $-1$ eV (weakly physisorbed) and below $-2$ eV (strongly chemisorbed). Hence, we obtained that the Rh–Sn$_3$C$_2$, Ru–Sn$_3$C$_2$, Pd–Sn$_3$C$_2$, Pd–Sn$_3$C$_2$, and Rh–Sn$_3$C$_2$ monolayers are good recoverable scavengers for the CO, CO$_2$, NO, NO$_2$, and SO$_2$ molecules. The current theoretical calculations provide new insight on the effect of TM adatoms on the structural, electronic, and magnetic properties of the Sn$_3$C$_2$ monolayer and different transition metal adatom as well as shed light on their application as gas sensors/scavengers.

Supplementary material for this article is available online

Keywords: gas sensing, 2D monolayer, transition metal adatom, density functional theory

(Some figures may appear in colour only in the online journal)
1. Introduction

The detection and sensing of organic, volatile, and toxic gaseous species at very low levels is essential in the monitoring, evaluation and setting standards for environmental protection [1, 2]. The discovery of new materials with high sensitivity to volatile and toxic gases, low cost and rapid response to different chemical species is an on-going effort using theoretical and experimental methods [2–8].

The discovery of 2D Ti3C2 nano-material produced at room temperature from the exfoliation of Ti3AlC2 have opened the way for synthesis of other 2D materials [9–11]. The Sn3C2 belongs to vast class of materials referred to as MXenes [12], which comprises of several layered ternary carbides and nitrides. These materials can be exfoliated or cleaved from the vast group of ternary carbides and nitrides materials with M_{n+1}AX [13–15] chemical formula (n = 1, 2, or 3; M = early transition metal; A = A-group (mostly groups 13 and 14) element, and X = C and/or N) or chemical synthesised. Recently, 3D framework [1] was fabricated for acetone, methanol and ethanol gas sensing. 2D V2CT, sensor devices consisting of single-/few-layer 2D V2CT, on polyimide film were fabricated and shown to detect both polar and nonpolar chemical species including hydrogen and methane with a very low limit of detection of 2 and 25 ppm, respectively, at room temperature (23 °C) [16]. 2D Ti3C2T, MXenes was fabricated and shown to possess high metallic conductivity for low noise and a fully functionalized surface for a strong signal. The Ti3C2T greatly outperform the sensitivity of conventional semiconductor channel materials for volatile organic compound with extremely low signal to noise ratio compared to the best known sensors [17]. The study also considered the role of CO2 gas and ethanol vapour on the interlayer swelling of Ti3C2T, MXene and its influence on the gas sensing performance [18]. Numerous investigations have been carried out on different MXenes as well as 2D materials as possible catalyst, support, battery material, etc [11, 18–24].

To the best of knowledge, no studies have been carried out on pristine or adatom Sn3C2 monolayer as a possible scrubber/ scavenger for these five common industrial exhaust gases, which are CO, CO2, NO, NO2 and SO2. The use of Sn and C atoms are the primary materials is motivated by the low cost of these materials.

The current study applied density functional theory calculation as implemented in the CASTEP code [25, 26] to investigate the effects and interactions of single adatom transition metal (TM = Cr, Mn, Fe, Mo, Ru, W and Os) on Sn3C2 monolayer with underlying hexagonal symmetry similar to Ti3C2 MXene monolayer as a scavenger of the CO, CO2, NO, NO2 and SO2 gaseous species. The introduction of dopant or adsorbate atoms have been shown to modulate the structural, electronic and optical properties of various host 2D materials [10, 27–34]. The use of adatoms on the Sn3C2 monolayer is applied in this study to understand the role of 3d and 4d transition metal adsorbates (where 3d = Fe, Co, Ni, Cu and 4d = Ru, Rh, Pd, Ag) on the Sn3C2 monolayer for scavenging and detection of light molecules in the atmosphere. Stronger molecular adhesion of all the molecules considered were observed in the presence of the 3d transition metals (Fe and Co), whereas all the considered 4d transition metals showed weaker molecular adhesion based on density functional theory calculations [35]. This implies that the Sn3C2 monolayer can be applied for the sensing and scavenging of the following gases: CO, CO2, NO, NO2 and SO2. The recovery time of these gases on the considered monolayers was presented to highlight their reusability. We obtained that the Rh–Sn3C2, Ru–Sn3C2, Pd–Sn3C2, Pd–Sn3C2, and Rh–Sn3C2 monolayers are good recoverable scavengers for CO, CO2, NO, NO2, and SO2 molecules.

2. Computational details

In this study, spin-polarised calculation density functional theory calculations [36, 37] were performed using CASTEP code [25, 38] as implemented in the Materials Studio package. The GGA-RPBE [39] exchange correlation functional and the on the fly generated ultra-soft pseudopotential was applied [40]. The hexagonal lattice representation of the Sn3C2 monolayer in the P-3M1 space group has been investigated in this study. The Tkatchenko–Scheffler method [41] for semi-empirical dispersion correction was applied to account for the van der Waals interaction in the system. Also, the self-consistent dipole correction was included in this study.

A k-point mesh separation of 0.07 Å−1, kinetic energy cut-off of 549.7 eV and 10−6 eV/atom convergence criteria for the calculated total energies was used to optimise the unit cell of Sn3C2 (where Sn = 3 and C = 2 atoms) monolayer (see figure 1). The forces in the Sn3C2 monolayer were converged up to 0.03 eV Å−1 for the full geometric optimisation. A 4 × 4 × 1 Sn3C2 super-cell (where Sn = 48 and C = 32 atoms) with vacuum distance of 18 Å was created from the unit cell and used for the adsorption energies calculation and the applied vacuum distance applied is appropriate to prevent interactions between periodic images [31]. The same convergence criteria used for the unit cell calculation was enforced for the super-cell calculation, however in this case only the atomic positions were optimised.

To determine the local stability of the Sn3C2 monolayer, the phonon frequencies at the high symmetry points (G-M-K-G) were calculated using density functional theory perturbation theory with the linear response approximation as implanted in the Materials Studio package [42]. The q-vector grid spacing for interpolation of 0.02 Å−1, convergence tolerance of 1.0−5 eV Å−2, and dispersion separation of 0.015 Å−1 is applied.

The calculated adsorption energy (E_{Ad–TM}) for the TM adatom on the Sn3C2 monolayer surface (TM-Sn3C2) was obtained using:

\[ E_{Ad–TM} = E_{TM–Sn3C2} - E_{Sn3C2} - \mu_{TM}. \]  

where \( E_{TM–Sn3C2} \) and \( E_{Sn3C2} \) are the calculated total energies of TM-Sn3C2 and pristine Sn3C2 super cells, respectively. \( \mu_{TM} \) is the chemical potential for the TM adatom. These were determined from their respective bulk unit cells.
The molecular adsorption energy ($E_{\text{Ad-Mol}}$) of each gaseous molecules on the pristine and TM-Sn$_3$C$_2$ monolayers was evaluated using the equation [43]:

$$E_{\text{Ad-Mol}} = E_{\text{TM-Sn$_3$C$_2$+Mol}} - E_{\text{TM-Sn$_3$C$_2$}} - \mu_{\text{Mol}}.$$  (2)

The $E_{\text{TM-Sn$_3$C$_2$+Mol}}$, $E_{\text{TM-Sn$_3$C$_2$}}$ and $\mu_{\text{Mol}}$ are total energies of the pristine or TM-Sn$_3$C$_2$ monolayers with the various molecules, total energies of the pristine or TM-Sn$_3$C$_2$ monolayers and the chemical potential of the various molecules considered. The $\mu_{\text{Mol}}$ is evaluated using the calculated total energy of the CO, CO$_2$, NO, NO$_2$ and SO$_2$ molecules. The stability of the TM-Sn$_3$C$_2$ monolayers considered was argued purely based on the formation energies due to the system size and the different configurations considered. This allows the computations to be tractable. This is in line with other previous studies [44–46].

### 3. Results and discussions

#### 3.1. Geometric, phonon properties, and electronic structure

The Sn$_3$C$_2$ monolayer was found to have a non-magnetic ground state with a formation energy of $-2.78$ eV. This formation energy of the Sn$_3$C$_2$ monolayer is calculated using the procedure given in previous studies [47]. The implication is that the formation of Sn$_3$C$_2$ monolayer is energetically favourable.

The calculated phonon dispersion plot and density of phonon states are presented in figures 2(a) and (b), respectively. No negative/imaginary phonon modes in the phonon dispersion plot and density of phonon states was observed in the Sn$_3$C$_2$ monolayer unit cell. This implies that the Sn$_3$C$_2$ monolayer is dynamically stable. The calculated phonon modes are comprised of two section, which ranges from 0 to 6 THz and 7 to 14 THz. The lower modes are governed by the Sn atoms whereas the higher modes are governed by the C atoms. This is consistent with previous studies [48, 49] which shows that heavy atoms make up the lower modes.

Next, the preferred adsorption site of TM adatoms on the pristine Sn$_3$C$_2$ super-cell surface was evaluated using Ru atom to test different possible sites. The different possible adsorption sites were considered and used to determine the preferential adsorption site (see figure 1 and S. table 10 (available online at stacks.iop.org/NANO/32/355502/mmedia)). In figure 1, three of the likely sites was indicated and several other sites was The adsorption energy ($E_{\text{Ad-TM}}$) for the TM adsorption onto the most favourable site is evaluated using the equation giving in equation (1). The preferred transition metal adatom location on the Sn$_3$C$_2$ monolayer is found to be the carbon hollow site, which is approximately in the centre of a triangle formed from three Sn atoms as presented in S. table 10 and figure 1. This site was used to study all the other adatoms considered as shown in table 1. The

Figure 1. Atomic structures of the pristine Sn$_3$C$_2$ monolayer and position of the likely TM adsorbate is indicated; where blue, and grey represents the Sn, and C atoms respectively.

### Table 1

<table>
<thead>
<tr>
<th>Adatom</th>
<th>EC</th>
<th>AR</th>
<th>$E_{\text{Ad-TM}}$</th>
<th>Tot Mag</th>
<th>TM-Sn$_x$</th>
<th>TM-Sn$_y$</th>
<th>TM-Sn$_z$</th>
<th>TM-Sn$_{avg}$</th>
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<td>Fe</td>
<td>[Ar]3d$^8$4s$^2$</td>
<td>156</td>
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<td>4.25</td>
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<td>2.9829</td>
<td>3.1658</td>
<td>3.2100</td>
<td>3.1196</td>
<td></td>
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<tr>
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<td>-1.41</td>
<td>3.0861</td>
<td>3.2748</td>
<td>3.2752</td>
<td>3.2120</td>
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<tr>
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<td>2.5864</td>
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<tr>
<td>Ru</td>
<td>[Kr]4d$^8$5s$^1$</td>
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<td>-8.25</td>
<td>3.86</td>
<td>2.5766</td>
<td>2.5770</td>
<td>2.5770</td>
<td>2.5768</td>
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<tr>
<td>Rh</td>
<td>[Kr]4d$^8$5s$^1$</td>
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<td>0.00</td>
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<tr>
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<td>3.0969</td>
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</tr>
<tr>
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<td>3.17717</td>
<td>3.1883</td>
<td>3.33316</td>
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</table>
The adsorption of all the considered TM adatoms on the Sn$_3$C$_2$ monolayer have negative $E_{\text{Ad-TM}}$, which implies that the formation of these structures is feasible. The $E_{\text{Ad-TM}}$ for the 4$d$ TM adatoms was found to be generally higher as compared to the 3$d$ TM adatoms. This result showed that the 4$d$ TM binds stronger to the Sn$_3$C$_2$ monolayer. The ground state of pristine Sn$_3$C$_2$ monolayer is obtained to be a non-magnetic metal, whereas the introduction of TM adatoms on the Sn$_3$C$_2$ monolayer surface (TM-Sn$_3$C$_2$) resulted in changes to the magnetic character. However, all the monolayers remain metallic. It is observed that the ground state structure of these TM adatoms (Fe, Co, Ni and Ru) on the Sn$_3$C$_2$ monolayer becomes magnetic as shown in table 1 with highest magnetisation obtained as a result of the Fe adatom on Sn$_3$C$_2$ monolayer, whereas the other TM adatoms (Cu, Rh, Pd, Ag) have non-magnetic ground state. This induced magnetisation can be attributed to the non-filled 3$d$ (Fe, Co and Ni) orbital as well as the odd filling of the 4$d$ Ru orbital in comparison with the other dopant atoms with filled 3$d$ (Cu) and 4$d$ (Pd and Ag), and even filling of the 4$d$ Rh orbital. The bond distance (TM-Sn$_3$, where $x = 1, 2$ and $3$) is the distance between the transition metal atom and the top-most tin metal and the average bond distance (TM-Sn$_{avg}$) between the adatoms and the Sn surface species was evaluated and presented in table 1. The shortest bond distances of 2.5379 Å and 2.5770 Å were obtained for the Rh and Ru adatoms on the Sn$_3$C$_2$ monolayer, whereas the largest bond distances of 3.2331 and 3.2120 Å were obtained for the Ag and Ni adatoms on the Sn$_3$C$_2$ monolayer. The calculated TM-Sn$_{avg}$ bond distance does not follow any specific trend with respect to the atomic radii. Also, going through the groups or periods, no specific trend was observed with respect to the evaluated bond distance.

### 3.2. Adsorption of different molecules on pristine and TM-Sn$_3$C$_2$ monolayer

The adsorption of the molecules (CO, CO$_2$, NO, NO$_2$, SO$_2$) on pristine Sn$_3$C$_2$ monolayer was evaluated by considering different sites and the lowest energy was taken as the preferred adsorption location. For the TM-Sn$_3$C$_2$ modified surface, the molecules were adsorbed on the adatom to evaluate the effect on adatom. The preferred adsorption location was used to evaluate the adsorption energies of the different molecules. The calculated adsorption energies of the CO, CO$_2$, NO, NO$_2$, SO$_2$ on the Sn$_3$C$_2$ monolayer and TM-Sn$_3$C$_2$ modified surface is presented in figure 3 and table 2.

For the molecules considered, the 3$d$ transition metal (Co, Cu, Fe and Ni) and Ru adatoms on Sn$_3$C$_2$ monolayer as well as pristine Sn$_3$C$_2$ monolayer have relatively lower $E_{\text{Ad-M}}$ –6 to −2 eV compared with the 4$d$ transition metal (Ag, Pd and Rh) adatoms on Sn$_3$C$_2$ monolayer with $E_{\text{Ad-M}}$ from −3 to −0.4 eV. The results indicate that the presence of 3$d$ transition metal (Co, Cu, Fe and Ni) and Ru adatoms on the Sn$_3$C$_2$ monolayer exhibit stronger sensing properties in comparison with the 4$d$ transition metal (Ag, Pd and Rh) adatoms on Sn$_3$C$_2$ monolayer. The implication of this observation is that Co, Cu, Fe and Ni and Ru on the Sn$_3$C$_2$ monolayer would bind release the adsorbed gaseous molecules tightly and not readily release the adsorbed gaseous molecules in comparison with the Ag, Pd and Rh on the TM-Sn$_3$C$_2$ surfaces. Thus, negative adsorption energies within the range of −1 to −2 eV are essential for good reusable gas scavengers. The desorption of the gaseous molecules would be further explored in detail in the next section. All the considered gaseous molecules on the pristine and TM doped Sn$_3$C$_2$ monolayer had the molecules adsorbed intact except for the NO molecule on the Fe−Sn$_3$C$_2$ monolayer. The NO molecule dissociates to the N and O atoms with a separation distance of 2.259 Å compared with an average bond distance of about 1.18 Å. The N and O atoms have a bond distance of 1.623 Å and 1.678 Å respectively with the Fe surface adatom.

We have observed from presented in figure 3 and table 2 that: (i) the Rh−Sn$_3$C$_2$ monolayer have comparable higher adsorption energies than the pristine and doped monolayer for the CO$_2$ and SO$_2$ molecules with adsorption energies of −0.49 and −1.31 eV, (ii) the Pd−Sn$_3$C$_2$ monolayer have comparable higher adsorption energies than the pristine and adatom Sn$_3$C$_2$ monolayer for the NO and NO$_2$ molecules with adsorption energies of −1.23 and −1.53 eV, and (iii) Ag−Sn$_3$C$_2$ monolayer have comparable higher adsorption...
molecule on the Ag surface. The relative difference in the adsorption energy for the CO molecule is negative, with adsorption energies within the range of -1.53 eV. These negative adsorption energies are essential for reusable gas scavengers.

The relative difference in the adsorption energy for the CO molecule on the Ag–Sn₃C₂ monolayer compared with the Rh–Sn₃C₂ is about 0.02 eV. Thus, the Rh–Sn₃C₂ monolayer might as well be suited for the use as a gas scavenger for the CO molecule as well as the CO₂. For one-time use materials, stronger adsorption and sensing of these gaseous molecules are paramount, therefore the 3d transition metal dopant atoms would be better suited than the suggested 4d transition metal dopant atoms. For reusability, weaker adsorption is paramount as demonstrated in previous studies [6]. Thus, the desorption of the gaseous molecules on the above suggested possible candidate monolayers is discussed.

### 3.3. Desorption of different gaseous molecules on pristine and TM-Sn₃C₂ monolayer

The pristine and TM adatoms on Sn₃C₂ monolayer adsorb the different gaseous molecules strongly to their surface of the structure. This strong binding observed on the surface demonstrate that the TM doped, and pristine Sn₃C₂ monolayer are applicable as sensors/scavengers for these gaseous molecules (CO, CO₂, NO, NO₂, SO₂). The energetics of the gaseous molecules show strong binding on the considered surfaces. The observed high adsorption energetics have a major drawback in terms of usage of these surfaces, where recovering the catalytic surface for subsequent use would result in longer recovery time (τ). The τ for the desorption of the gaseous molecules (CO, CO₂, NO, NO₂, SO₂) on pristine Sn₃C₂ monolayer was evaluated using the Arrhenius-type equation given below [2, 50, 51]:

\[
\tau = \nu_0^{-1} e^{(-E_a/k_B T)},
\]

where \( T \) is temperature, \( K_B \) the Boltzmann’s constant and \( (8.318 \times 10^{-3} \text{ kJ (mol}^\text{°K})^{-1}) \) \( \nu_0^{-1} \) is the attempt frequency \((10^{12} \text{s}^{-1})\).

The equation considers the relationship between the temperature and the rate constant of a given chemical reaction. The above expression is based on transition state theory and van’t Hoff–Arrhenius expression. Equation (3) shows an exponential relation between the recovery time and the calculated temperature. Thus, the Sabatier principle is of consequence, where a balance between the adsorption energy and recovery time is needed to have either an irreversible or reversible gas scavenger. Based on this, the optimal adsorption energy for reusable gas scavengers is between -1 and -2 eV.

In figure 4, the recovery time in log scale (base 10) for different adsorbed gases (CO, NO, NO₂, SO₂) as a function of different temperatures (298, 373 and 473 K) at the most optimal surfaces as found in section 3.2 is presented except for CO₂, whereas the recovery time as a function of
temperature for CO₂ is presented in figure 4. The optimal adsorption energy for reusable gas scavengers is between −1 and −2 eV. This would result in reasonable desorption time and temperatures. The NO₂ and CO molecules have similar adsorption energy, hence overlay on each other in figure 4 (see S. tables 8 and 9). The temperature range is essential to maintain the integrity of the Sn₃C₂ monolayer and prevent disintegration. For the CO₂ molecule adsorbed on the pristine and adatom Sn₃C₂ monolayers, the highest adsorption energy of ≈0.49 eV would result in desorption of the CO₂ molecule below room temperature and almost spontaneous (10⁻⁸ s). This implies that for practical application above room temperature this material is impractical. At room temperature (298 K) and boiling point of water (373 K), the time required for the desorption of the CO, NO, NO₂, and SO₂ molecules on the Ag–Sn₃C₂, Pd–Sn₃C₂, Pd–Sn₃C₂, and Ag–Sn₃C₂ monolayers respectively is relatively longer when compared with the 473 K temperature. Considering the NO molecule on the Pd–Sn₃C₂ monolayer as presented in figure 4 and table 3, the recovery time for the desorption of the molecule at room temperature is 5577, 179 805 s (∼10¹⁵). If the temperature of the Pd–Sn₃C₂ monolayer is increased to 473 K, the recovery time for the desorption of the NO molecule is 50.2 s (∼10²). This implies that the CO, NO, NO₂, and SO₂ molecules on the Ag–Sn₃C₂, Pd–Sn₃C₂, Pd–Sn₃C₂, and Ag–Sn₃C₂ monolayers can operate stably at 298 and 373 K temperatures. It is worth stating that the scavenging of these gaseous molecules should operate stably also at lower temperatures with desorption highly unlikely. However, at significantly higher temperatures (598 and 798 K), the desorption of these gases readily occurs based on equation (3).

Figure 5 shows the recovery time versus temperature for the CO₂ molecule adsorbed on the pristine and TM adatom Sn₃C₂ monolayers. For the Pd–Sn₃C₂, Rh–Sn₃C₂ and Ag–Sn₃C₂ monolayers, the adsorption energies (recovery time) are −0.49 eV, −0.51 eV and −0.90 eV respectively. This implies that the molecules are physisorbed and the desorption time is very low making these configurations not feasible as scavengers. The Ru–Sn₃C₂ and Cu–Sn₃C₂ monolayers with energy range between −1 and −2 eV would form better recoverable sensors/scavengers of CO₂ molecule as shown in S. table 2.

For the monolayer configurations with lower adsorption energies such as pristine Sn₃C₂, Ni–Sn₃C₂, Fe–Sn₃C₂, and Co–Sn₃C₂ the desorption of the adsorbed molecules (CO, CO₂, NO, NO₂ and SO₂) occurs at significantly higher temperatures (473 K and above) and long-time (10¹⁰–10³⁴ s) as presented in figure 6. The application of high temperature could lead to the degradation and de-activation of these monolayers. Hence, lower adsorption energy is proportional to exponentially prolonged desorption time and vice versa. Therefore, pristine and 3d TM-Sn₃C₂ monolayers would be applicable as highly sensitive irreversible sensors/absorbers rather than ideal reversible scavengers. Other materials have been investigated for the adsorption of these gases such as graphene [52], pristine and defective MoS₂ [53–57], pristine and defective MoSe₂ [4, 58], InN [59], borophene [60], etc [61–63]. The considered pristine and TM-Sn₃C₂ monolayer adds to this class of materials, which can be used to sense/scavenger gaseous molecules and offers different temperature regime as well as binding strength with varied applicability.

4. Conclusions

In the current study, density functional theory-based calculations were carried out to study the influence of different transition metal adatom on Sn₃C₂ monolayer towards the adsorption of the CO, CO₂, NO, NO₂, and SO₂ toxic gases. A predicted thermodynamic Sn₃C₂ monolayer was established using arguments based on the phonon frequencies and calculated formation energy. The calculated binding energies of the transition metal atoms (3d = Fe, Co, Ni, Cu and 4d = Ru, Rh, Pd, Ag) show that the various considered adatoms stably bind on the Sn₃C₂ monolayer.

The calculated adsorption energies of the CO, CO₂, NO, NO₂, and SO₂ molecules obtained on the pristine and TM-Sn₃C₂ monolayers are all negative. This implies that the considered configurations will bind the CO, CO₂, NO, NO₂, and SO₂ molecules stably. The TM (3d)-Sn₃C₂ monolayers were found to bind the CO, CO₂, NO, NO₂, and SO₂ molecules stronger compared with the TM (4d)-Sn₃C₂ monolayers.

The recovery time for the desorption of the molecules on the pristine and TM-Sn₃C₂ monolayers was evaluated using an Arrhenius-type equation. We determined that negative adsorption energies within the range of −1 to −2 eV for the gaseous molecules resulted in the desorption of the gaseous molecules at moderate time for slightly elevated temperatures ∼473 K. At adsorption energies of 0 to −1 eV, the gaseous species physisorbed. Thus, from the calculated recovery time, the desorption of the gaseous molecules occurs almost instantaneous, hence those TM-Sn₃C₂ monolayers would not be ideal as scavengers/sensors. We found that the Rh–Sn₃C₂, Ru–Sn₃C₂, Pd–Sn₃C₂, Pd–Sn₃C₂, and Rh–Sn₃C₂ monolayers
based on the adsorption energy and the recovery time would form good recoverable scavengers for the CO, CO₂, NO, NO₂, and SO₂ gaseous species.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Conflicts of interest

No conflicts of interest to declare.

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Nanotechnology 32 (2021) 355502
K O Obodo et al


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