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DFT-driven multitask deep learning for sulfur gas sensing and removal by transition metal phthalocyanines

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Abstract

Accurate prediction of both gas sensitivity and adsorption capacity is essential for developing high-performance sensing and purification materials for sulfur-based toxic gases. However, these two targets are governed by multiple interrelated physicochemical factors originating from both the sensing material and gas molecules, making it challenging for experimental approaches and traditional machine learning methods to simultaneously capture their shared physicochemical information and task-specific characteristics. Herein, we develop a multi-task deep learning (MTDL) framework that simultaneously learns and shares representations between sensitivity and adsorption tasks to elucidate their cooperative mechanisms in transition-metal phthalocyanines (TM/Pc). Integrated with density functional theory (DFT) calculations, the MTDL model enables joint prediction of adsorption energies (E_{ads}) and sensing responses (SR) toward H_2S , SO , SO_2 , and SO_3 , achieving improved predictive performance compared with single-task models. Model interpretability analysis reveals that the predictions are governed by a coherent combination of metal-centered electronic properties, substrate-level electronic structure descriptors, and gas-phase electronic characteristics, providing a mechanistic insight into how adsorption-desorption equilibria and charge redistribution collectively determine sensing performance. Overall, this study demonstrates that multi-task learning effectively bridges adsorption thermodynamics and gas sensing response, offering a generalizable and interpretable strategy for AI-driven design of multifunctional gas-sensing and purification materials.

Keywords: Multitask deep learning, Gas sensitivity, Adsorption, Transition-metal phthalocyanine, Density functional theory

Highlights

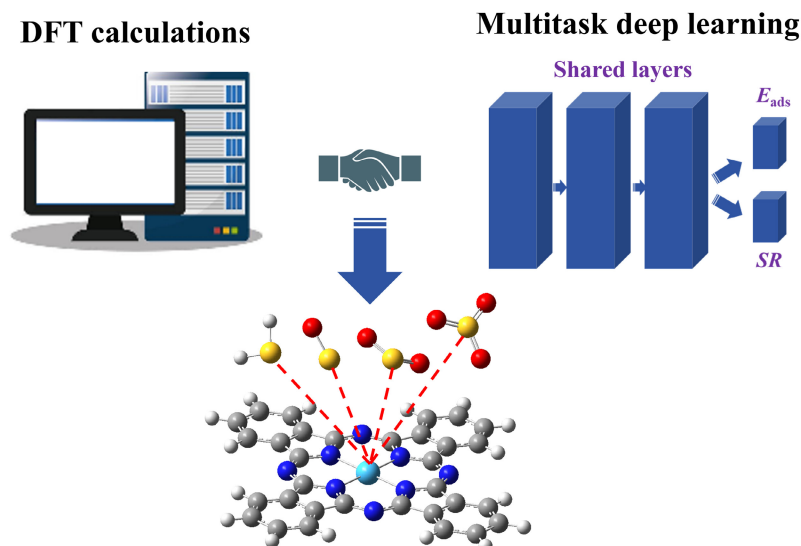
- The mechanisms underlying TM/Pc effectiveness as sulfur-based gas binders or absorbers were studied.
- Structure-property relationships of TM/Pc were established with the adsorption of sulfur-based gas.
- A multitask deep learning model was used to simultaneously predict gas sensing and gas capture ability.
- Key factors governing sensing performance were identified from both TM/Pc and gas properties.

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Graphical abstract



Introduction

Rapid industrialization has significantly exacerbated air pollution in recent years, posing serious threats to human health and environmental integrity. Sulfur-based gases, major contributors to air pollution, are emitted from various sources, including the combustion of fossil fuels and industrial wastewater emissions^[1]. Among these, hydrogen sulfide (H_2S) is a highly poisonous and flammable gas, with a safe exposure limit of less than 15 minutes at concentrations as low as 5 ppm^[2]. Sulfur oxide (SO) readily transforms into sulfur dioxide (SO_2), which can induce respiratory inflammation by reacting with atmospheric radicals or ozone^[3]. At concentrations above 10 ppm, SO_2 can cause respiratory diseases and eye burns, and exposure to levels of 20 ppm or higher may lead to lung failure or death. Moreover, H_2S and SO_2 are common byproducts of sulfur hexafluoride (SF_6) decomposition, a critical factor in assessing the safety of gas-insulated switchgear^[4–6]. Sulfur trioxide (SO_3), another toxic compound, is a primary component of acid rain^[7]. Consequently, the effective monitoring and removal of sulfur-based gases are imperative for both human health and ecological well-being.

Gas sensors are increasingly recognized for their potential to detect various volatile organic compounds (VOCs). The performance of these sensors is largely determined by their core component, the sensing material. Phthalocyanine (Pc), a p-type semiconductor, has shown promise as a gas-sensing material because of its high surface area, distinct electronic structures, and excellent stability^[8]. Recent advancements have enabled the synthesis of high-quality, large-area transition metal phthalocyanine (TM/Pc) materials that exhibit excellent gas-sensing performance^[9,10]. For instance, a reported Ni/Pc-based sensor exhibits exceptional selectivity towards H_2S and NO within just 1.5 minutes of exposure^[11]. A fluorinated Fe/Pc nanowire sensor was found to respond to NH_3 concentrations as low as 5 ppb^[12]. A 2D bimetallic CuNi/Pc-based covalent organic framework has been developed, exhibiting high sensitivity to NO_2 at 50 ppb^[13].

Despite the potential of TM/Pc materials, identifying optimal compositions for specific gases through trial and error is challenging due to the vast number of possible TM ions. Fortunately, integrating machine learning with DFT calculations offers a powerful approach for high-throughput screening of materials^[14,15]. DFT

calculations provide crucial insights such as density of states, energy gaps, and electronic distributions^[16], while machine learning techniques establish quantitative structure-property relationships, using specific data to predict material performance^[17,18]. However, despite these successes, achieving the synergistic optimization of multiple objectives remains a formidable challenge. In gas-sensing materials, SR determines the sensor's responsiveness and detection limit, while E_{ads} governs the interaction strength between gas molecules and active sites, influencing both selectivity and recovery behavior. Striking an appropriate balance between these two factors is essential yet difficult, as enhancing one often compromises the other. Traditional single-task machine learning models, which focus on a single property at a time, cannot effectively leverage the shared physicochemical information between sensing performance and adsorption behavior while preserving the task-specific information required for each prediction task, leading to suboptimal or biased material design outcomes. In contrast, MTDL provides an effective framework to simultaneously learn and exploit the shared and task-specific representations underlying these interdependent properties^[19], enabling more balanced and physically consistent optimization of gas-sensing materials.

This study uses DFT to investigate the stability and electronic properties of 28 TM/Pc substrates and four sulfur-based gases (H_2S , SO, SO_2 , and SO_3), yielding 78 adsorption systems. We systematically analyze the sensing properties of ideal TM/Pc materials for sulfur gases, considering factors such as natural bond orbital charge, electrical conductivity, and charge density differentials. Furthermore, a MTDL framework was established to jointly predict SR and E_{ads} , allowing the model to learn shared physicochemical representations while preserving task-specific information for each prediction task. This research provides a theoretical and data-driven foundation for the rational design of high-performance TM/Pc materials for gas detection and purification applications.

Materials and methods

DFT calculations

All the DFT calculations in this study were performed at room temperature (298 K) using the Gaussian 16 software^[20] and visualized

with virtual molecular dynamics software^[21]. The ω B97XD functional^[22] was used for all structural optimization and frequency calculations at the 6–311G (d,p)^[23] basis set for nonmetal atoms and LANL2TZ^[24] basis set for metal atoms, which can provide reliable results^[25–28]. In addition, independent gradient model based on Hirshfeld partition (IGMH), electrostatic potential (ESP), quantum theory of atoms in molecules (QTAIM), and density of state (DOS) were analyzed using the Multiwfn program^[29].

The interaction strength between the target gas and the TM/Pc was evaluated by calculating E_{ads} based on Eq. 1:

$$E_{\text{ads}} = E_{\text{Complex}} - (E_{\text{TM/Pc}} + E_{\text{Gas}}) + E_{\text{BSSE}} \quad (1)$$

where E_{Complex} , E_{Gas} , and $E_{\text{TM/Pc}}$ denote the total energies of the gas-TM/Pc complex, isolated gas molecule, and pristine TM/Pc, respectively. The basis set superposition error (E_{BSSE}) problem was considered by using counterpoise correction.

The charge redistribution after gas adsorption was considered by calculating the charge density difference (CDD), as described in Eq. 2:

$$\Delta\rho = \rho_{\text{Complex}} - \rho_{\text{TM/Pc}} - \rho_{\text{Gas}} \quad (2)$$

where ρ_{Complex} , ρ_{Gas} , and $\rho_{\text{TM/Pc}}$ are the charge densities of the gas-TM/Pc complex, isolated gas molecule, and pristine TM/Pc, respectively.

The stability of TM/Pc was evaluated through the binding energy (E_{bind}), which is defined as the following Eq. 3:

$$E_{\text{bind}} = E_{\text{TM/Pc}} - E_{\text{Pc}} - E_{\text{TM}} \quad (3)$$

where $E_{\text{TM/Pc}}$, E_{TM} , and E_{Pc} are the total energies of TM/Pc, isolated TM atom, and pristine Pc, respectively. TM/Pc with negative values can be regarded as thermodynamically stable.

To further explore the sensing ability of TM/Pc towards sulfur based gases, SR was calculated by the following Eq. 4:

$$SR = \left(\frac{1}{\sigma_{\text{Complex}}} - \frac{1}{\sigma_{\text{Substrate}}} \right) / \frac{1}{\sigma_{\text{Substrate}}} \quad (4)$$

where $\sigma_{\text{Substrate}}$ and σ_{Complex} are electrical conductivity of the isolated substrate and its adsorption systems, respectively.

The electrical conductivity was determined using the following Eq. 5:

$$\sigma = AT^{3/2} \exp\left(\frac{-E_g}{2KT}\right) \quad (5)$$

where A is a certain constant, and E_g represents the energy gap.

Single task machine learning

Herein, four machine learning algorithms: Support Vector Machine (SVM)^[30], eXtreme Gradient Boosting (XGBoost)^[31], Gradient Boosted Decision Trees (GBDT)^[32,33], and Random Forest (RF)^[34] were used to predict the E_{ads} and SR of 78 gas-TM/Pc systems. E_{ads} was used to develop regression models, whereas SR was formulated as a binary classification task using a threshold value of 100 to distinguish high-performance from low-performance sensing materials. Because the SR values span more than 22 orders of magnitude, direct regression is highly susceptible to extreme values. Therefore, a classification formulation was adopted to distinguish high-performance from low-performance sensing materials. The threshold of 100 provides a nearly balanced class distribution while representing a more stringent criterion than the threshold of 0.5 adopted in a previous study^[35], thereby prioritizing materials with truly outstanding sensing performance. This resulted in 38 high-response samples (label = 1) and 40 low-response samples (label = 0). Four types of features were selected for subsequent machine learning and deep learning modeling: (i) TM atom features of TM/Pc; (ii) adsorption atom features

of the gas molecule; (iii) systematic features of TM/Pc; (iv) systematic features of the gas molecule. These features are generated from simple DFT calculations or collected from the Periodic Table of Elements. The detailed physical interpretations and corresponding values of the input features are listed in [Supplementary Tables S1–S5](#). The original dataset was randomly partitioned into a training set (62 samples) and a test set (16 samples) at an approximately 4:1 ratio. Five-fold cross-validation was performed on the training set to ensure robust model evaluation. All machine learning models were built using the Scikit-Learn package (version 1.1.3).

To evaluate the reliability of the machine learning regression model, the coefficient of determination (R^2), root mean square error ($RMSE$), and mean absolute error (MAE) were calculated by the following Eqs. 6–8:

$$R^2 = \frac{\sum_{i=1}^n (y_i^{\text{DFT}} - y_i^{\text{pred}})^2}{\sum_{i=1}^n (y_i^{\text{DFT}} - \bar{y}^{\text{DFT}})^2} \quad (6)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_i^{\text{DFT}} - y_i^{\text{pred}})^2}{n}} \quad (7)$$

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i^{\text{DFT}} - y_i^{\text{pred}}| \quad (8)$$

where, y_i^{DFT} and y_i^{pred} indicate the calculated value and predicted value, respectively, and $\bar{y}^{\text{DFT}}$ represents the average value.

The performance of the classification models was evaluated using accuracy, F1-score, and recall as metrics (Eqs. 9–11):

$$\text{Accuracy} = \frac{TP + TN}{TP + TN + FP + FN} \quad (9)$$

$$\text{Recall} = \frac{TP}{TP + FN} \quad (10)$$

$$\text{F1-score} = \frac{2TP}{2TP + FP + FN} \quad (11)$$

where TP, TN, FP, and FN denote true positives, true negatives, false positives, and false negatives, respectively.

Multiple task deep learning

A multitask deep learning (MTDL) framework was constructed to simultaneously predict E_{ads} and SR , aiming to exploit shared physicochemical representations while preserving task-specific information within a unified learning framework. The network adopts a shared-task-specific hierarchical architecture, where three fully connected layers with progressively reduced dimensionality serve as a shared backbone to extract high-level latent features, employing LeakyReLU activation and a stepwise Dropout strategy to enhance training stability and generalization ([Fig. 1](#)). Task-specific branches were then introduced, with a regression head consisting of two fully connected layers with a fixed Dropout rate of 0.5 for E_{ads} prediction, and a lightweight classification head using two fully connected layers with a Sigmoid activation function for SR classification. Model training was performed using five-fold stratified cross-validation combined with an early stopping mechanism (maximum 2000 epochs) to prevent overfitting, while Mixup data augmentation was applied in the feature space to improve robustness against noise and outliers. The optimization objective was defined by a dynamically weighted composite loss function (Eq. 12):

$$L_{\text{total}} = \alpha \cdot L_{\text{CE}} + \beta \cdot L_{\text{MSE}} \quad (12)$$

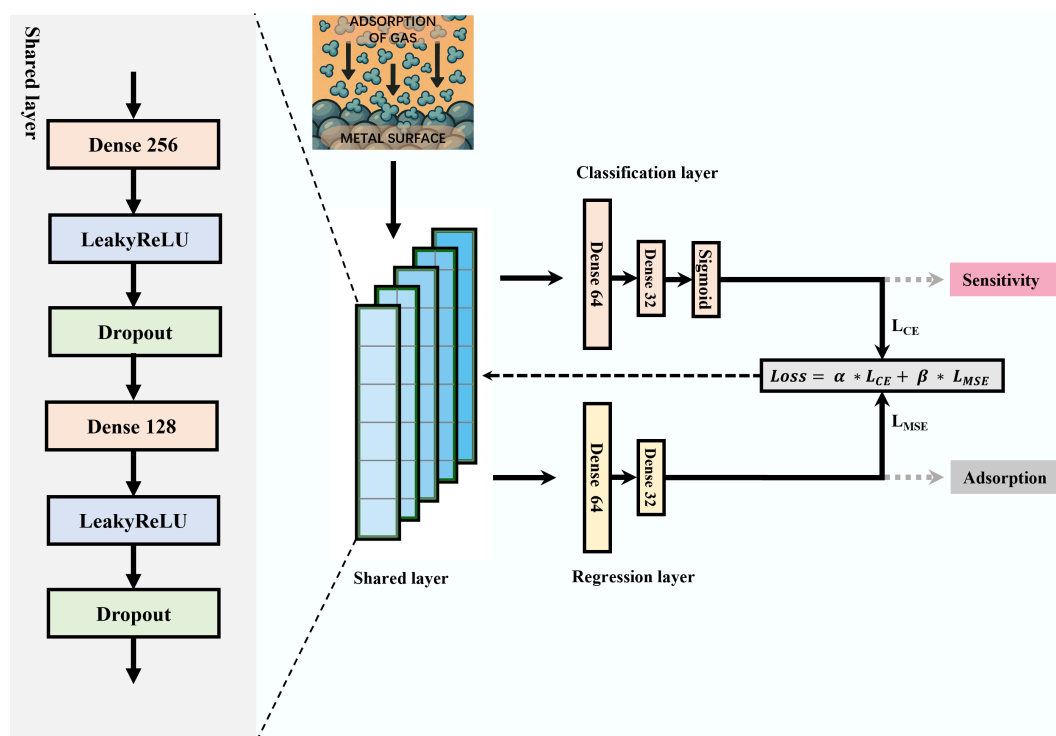


Fig. 1 Schematic illustration of the MTDL framework for joint prediction of SR and E_{ads} .

where L_{MSE} denotes the mean squared error (MSE) for E_{ads} prediction and L_{CE} represents the cross-entropy loss for SR classification. The task-weighting coefficients α and β were determined through a sensitivity analysis by systematically varying their values and evaluating the corresponding performance of both prediction tasks (Supplementary Table S6). The optimal coefficients ($\alpha = 0.4$, $\beta = 0.6$) were selected because they provided the best balance between E_{ads} regression and SR classification. To ensure experimental rigor, all hyperparameters were determined exclusively via grid search on the five-fold cross-validation performance on the training set. No test set information was utilized during this process, thereby preventing data leakage and ensuring an objective evaluation of our framework. The deep learning model was constructed and trained using the PyTorch framework (version 2.0.1).

Results and discussion

Stability and electronic properties of TM/Pc

The geometric structure of TM/Pc is depicted in Fig. 2a. Twenty-eight different potential TM/Pc materials are obtained by embedding close-packed 3d, 4d, and 5d TMs (Fig. 2b). As shown in Supplementary Figs. S1–S3, there are no negative vibrational frequencies, which means that all the optimized TM/Pc are minima and stable. After full relaxation optimization, the Cd, Hf, Sc, Ta, Ti, and Y atoms protruded from the Pc plane (Fig. 3a1), which are classified as the protrusion type. For Nb/Pc, Re/Pc, Ru/Pc, W/Pc, and Zr/Pc, two benzene rings move upwards, and the other two benzene rings move downwards (Fig. 3b1), which is classified as the butterfly type. The other TM atoms embedded in Pc exhibit a coplanar structure (Fig. 3c1).

The bond lengths between the TM atoms (V, Ti, Sc, Zn, Cr, Fe) and N atoms are 1.98, 1.99, 2.08, 2.00, 1.95, and 1.94 Å, respectively, which are consistent with the published theoretical results^[36,37]. As seen in Fig. 4a, the calculated TM–N bond length is shorter than the sum of their covalent radii^[38], indicating that stable bonds can be

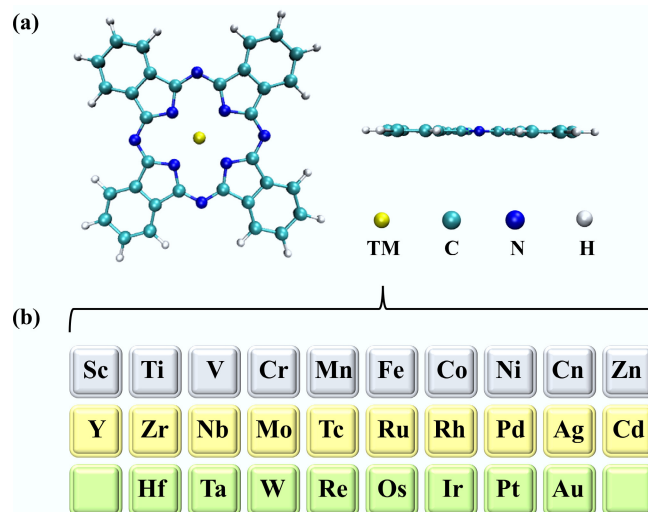


Fig. 2 Top and side views of the geometric structures of (a) TM/Pc and (b) 28 TM atoms embedded in Pc.

formed between the TM and the N atoms. Figure 4b displays the E_{bind} for all 28 TM/Pc, and corresponding values are listed in Supplementary Table S7. The E_{bind} values are in the range of -3.55 eV (Ag/Pc) to -11.75 eV (Hf/Pc), suggesting that 28 TM atoms can be effectively embedded into Pc, which ensures their high thermodynamical stability. To explore charge distribution and bonding characteristics between the TM and the N atoms, the electron localization function was evaluated by Multiwfn wave function analysis. Three representative TM/Pc were selected (Hf/Pc, Ru/Pc, and Ag/Pc with the highest, moderate, and lowest E_{bind} values). Figure 3a2 shows a higher ELF (Electron Localization Function) value of approximately 0.5 between the Hf and N atoms, indicating some degree of

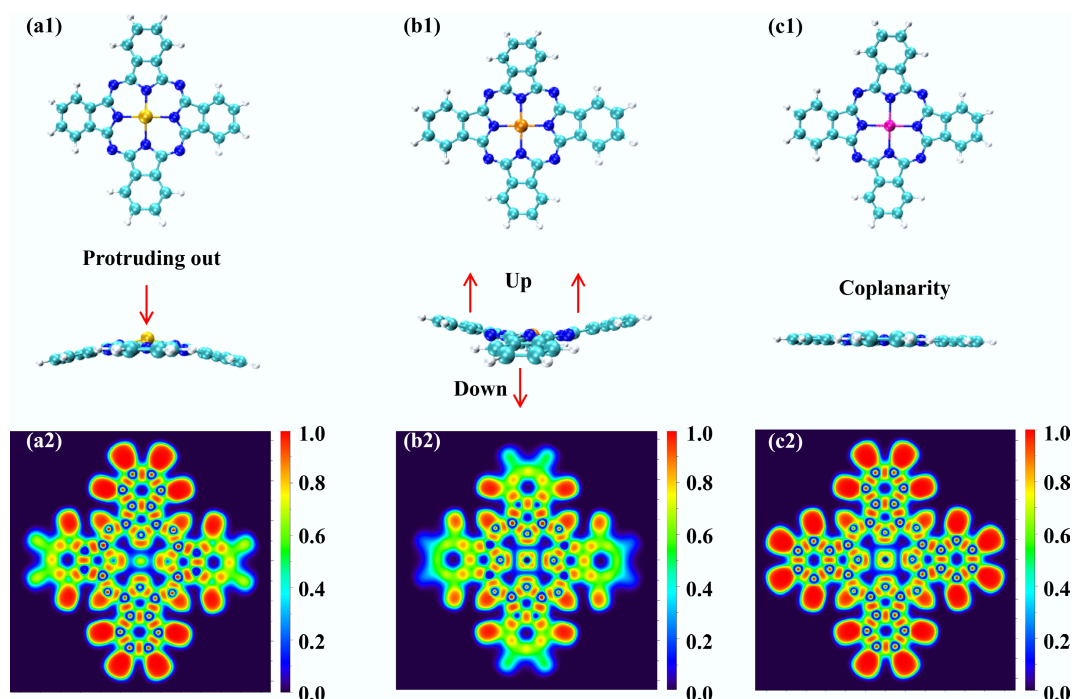


Fig. 3 Three representative geometric optimization models (up) and electron localization functions (down): (a1–a2) Hf/Pc, (b1–b2) Ru/Pc, and (c1–c2) Ag/Pc.

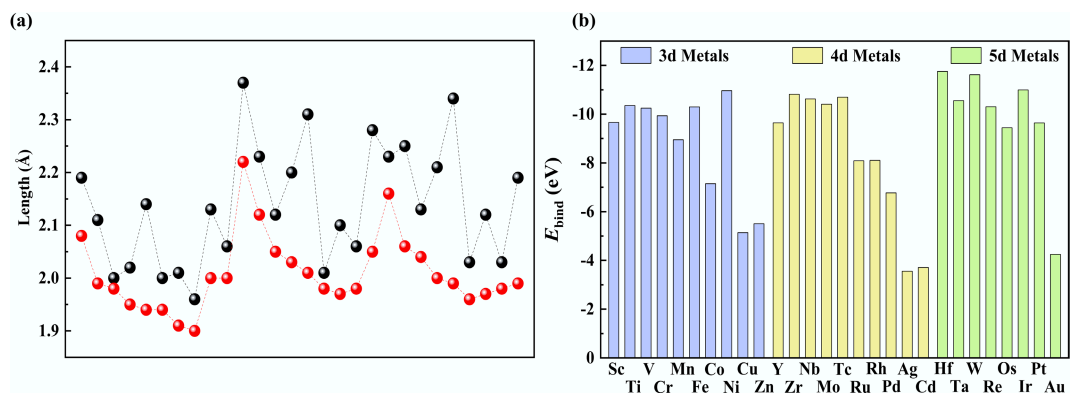


Fig. 4 (a) Covalent radii (black sphere) and bond length (red sphere) between TM and N atoms. (b) Binding energy (E_{bind}) of TM-embedded Pc.

electron localization, which may be an essential reason for its highest E_{bind} . As shown in Fig. 3b2–c2, the blue and dark blue regions appear between the Ru, Ag, and N atoms, which indicates that there is a weak interaction compared with that of Hf/Pc.

Figure 5 plots the density of states (DOS) of the 5d TM-decorated Pc to understand the electronic properties of TM-decorated Pc compared with pristine Pc. It can be seen that new energy states are introduced after embedding the 5d TM in Pc. Compared with pristine Pc, the HOMO of 5d TM/Pc appears shifted to higher energy, while the LUMO appears shifted to a lower energy, which leads to a smaller energy gap. 3d TM- and 4d TM-decorated Pc also exhibit similar behavior (Supplementary Figs. S4 and S5). Therefore, the electron transfer from HOMO to LUMO becomes easier after embedding TM.

ESP analysis can provide insights into charge distribution characteristics and potential interaction sites^[37,38]. Blue, white, and red on the ESP maps represent the electron-rich, neutral, and electron-deficient regions, respectively. As depicted in Fig. 6, negative potential regions are observed near Rh, Co, Pt, Cu, Pd, W, Os, Ir, Ru, and Ni

atoms, with corresponding values ranging from -0.01 (Ni/Pc) to -1.34 eV (Os/Pc). Other TM atoms exhibit a positive potential (Supplementary Fig. S6), with the most positive potential at the Ta atom (7.95 eV), and Re/Pc exhibits the lowest positive potential of 0.24 eV. The potential distribution of sensing materials is influenced by different TM atoms, which is beneficial for the effective regulation of adsorption performance based on our previous research^[39,40].

Supplementary Figure S7 illustrates the relaxed geometries of the four sulfur gases and their related ESP. The S–H bond length and H–S–H bond angle of H_2S are 1.34 Å and 92.66°, respectively. The structure of SO_2 is similar to H_2S , but the bond length and bond angle are slightly increased due to the larger radius of the O atom. SO_3 and SO_2 exhibit similar bond lengths and bond angles, but their S–O bond lengths are shorter than that of SO (1.49 Å). These findings are consistent with previous studies^[41,42]. For SO, SO_2 , and SO_3 , the positive potential is around the S atom, with values of 1.46, 1.50, and 2.52 eV, respectively, while the O atom exhibits a negative potential with corresponding values of -1.02 , -0.99 , and -0.56 eV,

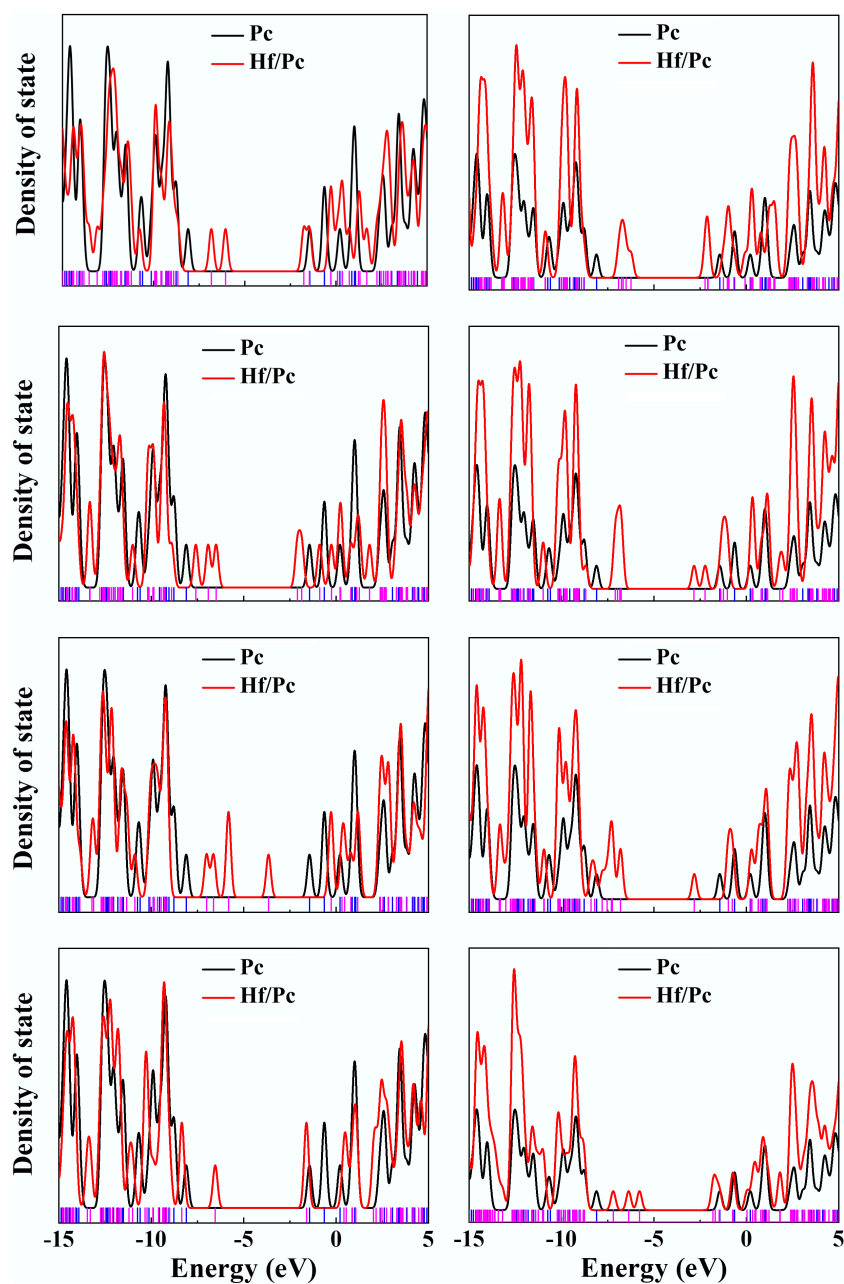


Fig. 5 Density of states of Pc and 5d transition-metal-embedded Pc.

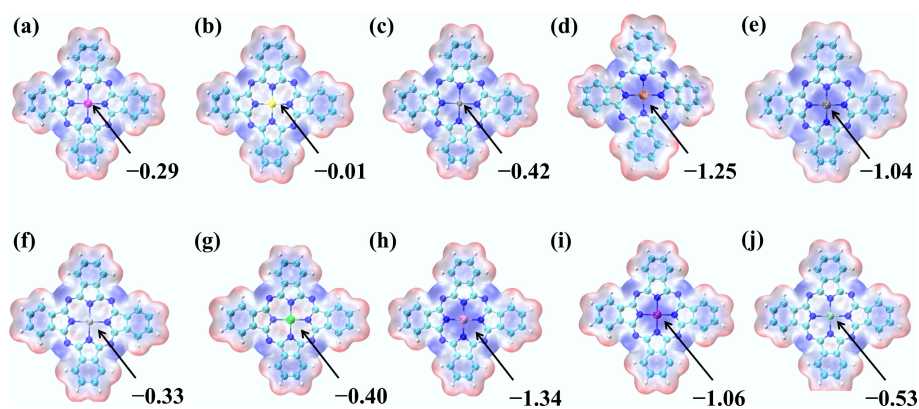


Fig. 6 ESP surfaces of (a) Co/Pc, (b) Ni/Pc, (c) Cu/Pc, (d) Ru/Pc, (e) Rh/Pc, (f) Pd/Pc, (g) W/Pc, (h) Os/Pc, (i) Ir/Pc, and (j) Pt/Pc. The unit of the data is eV.

respectively. The positive and negative potentials of H₂S are located near the H (1.07 eV) and S (−0.80 eV) atoms, respectively. This phenomenon is attributed to the higher electronegativity of S than of the H atom.

Adsorption of sulfur gases on TM/Pc

The recovery time (τ) can reflect the reusability of the sensor, which is an important indicator for determining its practicality. It can be calculated by the following equation:

$$\tau = \nu_0^{-1} \exp\left(-\frac{E_{\text{ads}}}{K_B T}\right) \quad (13)$$

where T is the temperature, ν_0 is attempt frequency, K_B is the Boltzmann's constant. Based on Eq. 13, a larger E_{ads} will prevent gas desorption from the substrate surface, which limits the sensor's reusability period. A smaller adsorption energy is insufficient to generate a recordable electrical signal for effectively detecting target gases. Therefore, gas sensors with appropriate recovery time are desirable. Generally, the appropriate recovery time should be within the range of a few seconds to about 1,000 s^[43]. According to previous work, in order to achieve the ideal recovery time, the range of the adsorption energy should be between −1 eV and −0.78 eV^[35,44].

Adsorption behavior and charge transfer analysis

Based on previous research, various potential materials were selected from 28 TM/Pc for adsorbing different sulfur gases. All initial adsorption configurations were constructed according to the potential interaction sites identified from ESP analysis. The E_{ads} values are plotted in Fig. 7,

and the corresponding values are summarized in [Supplementary Table S8](#). Strong adsorption strength is a necessary condition for a superior adsorbent. Zr, Mo, Ru, Hf, Ta, and Os atoms embedded in Pc exhibit intense adsorption energy for SO in the range of −5.93 to −4.79 eV. For SO₂ gas, ten TMs (Sc, Ti, Y, Zr, Nb, Ru, Hf, Ta, W, and Os) embedded in Pc exhibit larger adsorption energy in the range of −4.41 to −2.67 eV, making them suitable for use as gas removers or adsorbers. The ideal gas-sensing TM/Pc for sulfur gases, namely, H₂S-Ti/Pc, H₂S-Cr/Pc, SO-Fe/Pc, and H₂S-Fe/Pc, and their corresponding E_{ads} values are −1.01, −0.92, −0.90, and −0.84 eV, respectively. Previous studies have shown that applying an electric field can alter the adsorption strength^[45–47]. Therefore, the adsorption energy close to the maximum and minimum limits is also considered, including H₂S-Y/Pc (−0.72 eV), H₂S-Sc/Pc (−0.75 eV), SO₃-Cd/Pc (−1.06 eV), H₂S-Tc/Pc (−1.08 eV), SO₃-Os/Pc (−1.09 eV), and SO-Zn/Pc (−1.10 eV), and their corresponding adsorption energies under the electric field are shown in [Figs. 7c](#) and [7d](#). The adsorption energy of SO₃-Cd/Pc, SO₃-Os/Pc, and SO-Zn/Pc gradually increases with the electric field changes from −0.006 to +0.006 a.u., whereas the adsorption energy of H₂S-Y/Pc, H₂S-Sc/Pc, and H₂S-Tc/Pc gradually decreases, except for that of H₂S-Y/Pc under an electric field of −0.006 a.u.. Some adsorption energy values that meet the ideal recovery time criteria are marked with red boxes in [Fig. 7](#), and corresponding values are summarized in [Supplementary Table S9](#).

The most stable structures of H₂S-Fe/Pc, SO-Fe/Pc, H₂S-Cr/Pc, and H₂S-Ti/Pc are depicted in [Fig. 8a1–a4](#). It is evident that the S atom of H₂S is captured near the doping site, SO is captured by the doping site and the N atom. These adsorption systems have suitable adsorption distances ranging from 1.97 to 2.51 Å. [Supplementary Figure S8](#) illustrates the relaxed geometries of the other six

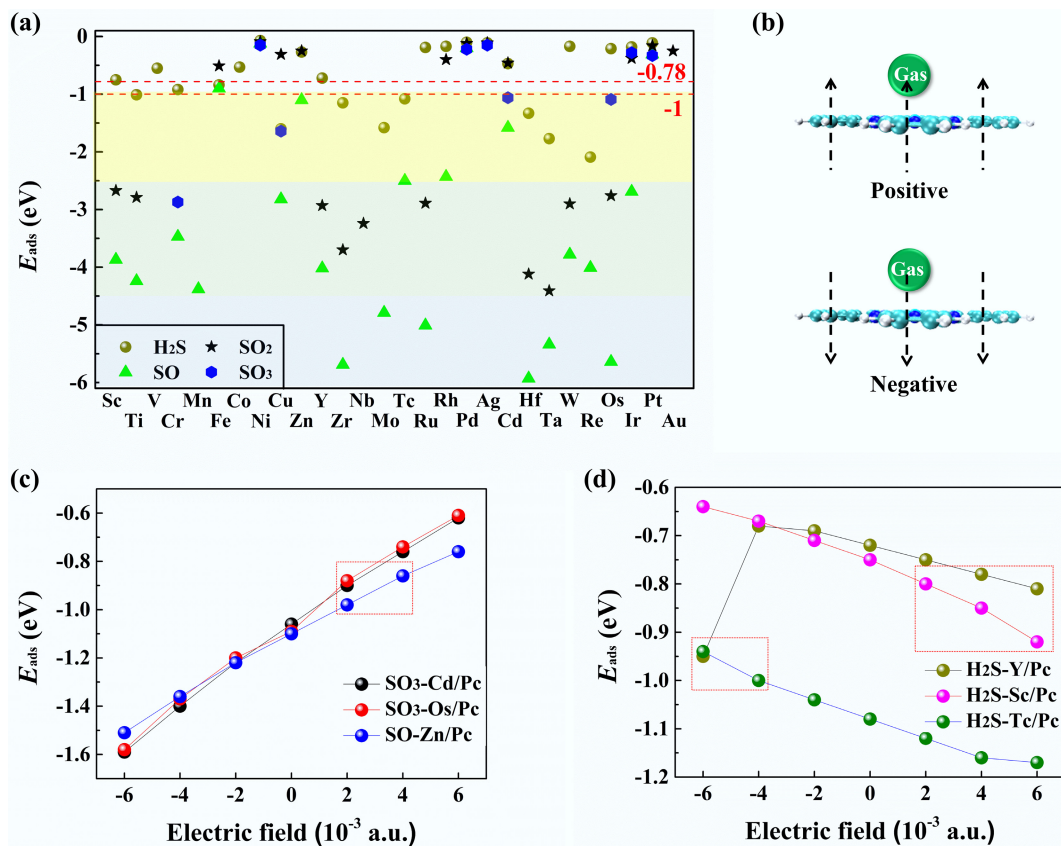


Fig. 7 (a) E_{ads} of sulfur gases on the transition-metal-embedded Pc; (b) direction of the applied electric field; (c)–(d) adsorption energy of SO₃-Cd/Pc, SO₃-Os/Pc, SO-Zn/Pc, H₂S-Y/Pc, H₂S-Sc/Pc, and H₂S-Tc/Pc under the applied electric field.

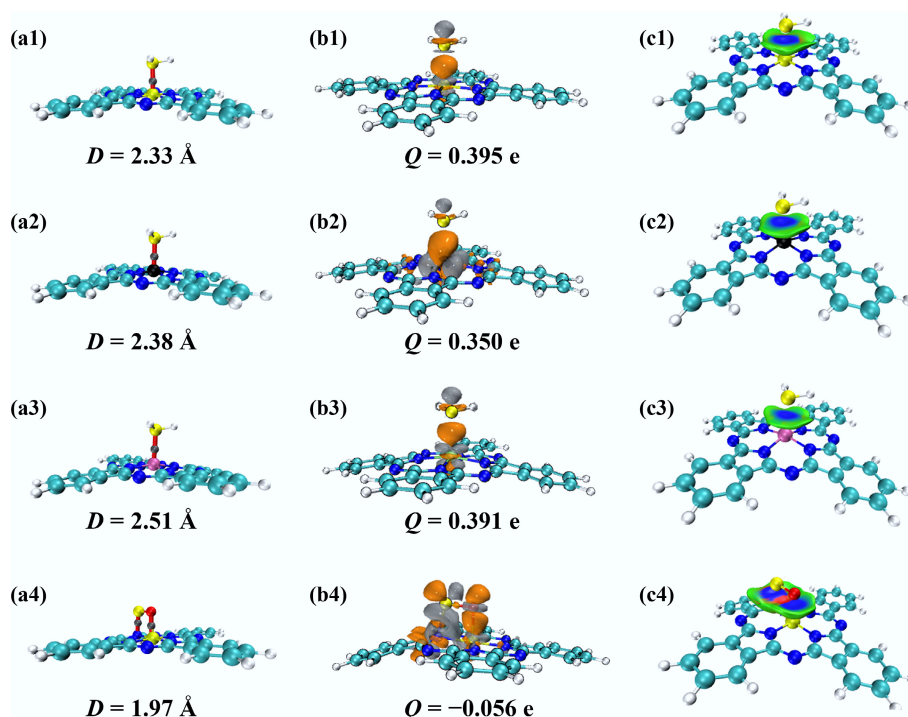


Fig. 8 Adsorption configuration (left column), CDD maps (middle column), and IGMH (right column) of (a1–c1) H₂S-Fe/Pc, (a2–c2) H₂S-Cr/Pc, (a3–c3) H₂S-Ti/Pc, and (a4–c4) SO-Fe/Pc complexes, respectively. The isosurface value is set to 0.003 e/Å³. Gray sphere and red line between residue pairs denote bond critical points (3, –1) and bond paths, respectively.

adsorption systems under the electric field. Electric fields have no significant effect on geometric structures. It is worth noting that H₂S, SO, and SO₃ are captured near the doping site and by nearby N and C atoms under the electric field. H₂S-Y/Pc has a relatively long adsorption distance of about 3 Å among the six adsorption systems.

To observe the characteristics of charge transfer, the CDD of the adsorption system is depicted in Fig. 8b1–b4. Orange (silver) region indicates electron accumulation (depletion). For H₂S adsorption systems, electron depletion appears on the H₂S molecule, while accumulation mainly occurs on the Fe, Cr, and Ti atoms and the interface. For the SO-Fe/Pc complex, electron depletion (accumulation) is mainly located on Fe/Pc (SO molecule). The natural bond orbital (NBO) analysis quantitatively confirmed this charge distribution. The H₂S molecule acts as an electron donor and transfers 0.395, 0.350, and 0.391 e to Fe/Pc, Cr/Pc, and Ti/Pc, respectively. The SO molecule attracts 0.056 e from the Fe/Pc. The results are consistent with CDD analysis. Supplementary Figure S9 illustrates the CDD of the other six adsorption systems under the electric field. SO₃ and SO molecules attract electrons from Os/Pc, Zn/Pc, and Cd/Pc. In contrast, H₂S acts as the donor and transfers electrons to Y/Pc, Sc/Pc, and Tc/Pc, respectively.

Analysis of interaction characteristics

IGMH is used to analyze the type of interaction between TM/Pc and sulfur-based gases by generating isosurfaces of different colors, such as strong attraction (blue color) and weak van der Waals interaction (green color). As shown in Fig. 8c1–c4, the strong attractive interaction (blue patches) is present between the S atom of H₂S gas and the TM atom of TM/Pc. It is worth noting that two blue patches can be found between SO and Fe/Pc. Under the electric field, a light blue region appears between H₂S gas and Y/Pc (Supplementary Fig. S10), indicating a relatively weak interaction strength compared with other adsorption systems. Two strong adsorption sites (dark blue isosurface) exist between SO, SO₃, Zn/Pc, and Cd/Pc, indicating relatively strong interaction between adsorbed atoms and TM atoms.

More detailed interaction characteristics can be found through QTAIM analysis. Figure 8a1–a4 illustrates bond paths and corresponding critical points of H₂S-Fe/Pc, SO-Fe/Pc, H₂S-Cr/Pc, and H₂S-Ti/Pc. The topological parameters, including Laplacian of total electron energy density $H(r)$, Lagrangian kinetic energy $G(r)$, potential electron energy density $V(r)$, and electron density $\nabla^2\rho(r)$, are listed in Table 1. According to Bader theory, $\nabla^2\rho(r)$ and $H(r) < 0$ denote the covalent interaction, $\nabla^2\rho(r) > 0$ and $H(r) < 0$ indicate partially covalent interaction, and the non-covalent character is defined when $\nabla^2\rho(r)$ and $H(r) > 0$ ^[48–50]. It can be shown in Table 1 that all

Table 1 Topological parameters at the bond critical points of the selected bonds for adsorption systems

System	Bond	$\nabla^2\rho(r)$	$V(r)$	$G(r)$	$H(r)$	$G(r)/ V(r) $
H ₂ S-Fe/Pc	S–Fe	0.2678	–0.0789	0.0729	–0.0060	0.9239
H ₂ S-Cr/Pc	S–Cr	0.1959	–0.0646	0.0568	–0.0078	0.8792
H ₂ S-Ti/Pc	S–Ti	0.1356	–0.0483	0.0411	–0.0072	0.8509
SO-Fe/Pc	O–Fe	0.4564	–0.1255	0.1198	–0.0057	0.9545
	S–N	0.0024	–0.1183	0.0594	–0.0589	0.5021

bond critical points exhibit a partially covalent nature. This adsorption characteristic can effectively balance adsorption and desorption properties. The results obtained can be further confirmed using the $G(r)/|V(r)|$. The type of interactions is non-covalent and partial covalent when the value is greater than 1, and between 1 and 0.5, respectively^[51,52]. The ratio of $G(r)/|V(r)|$ further confirms their partially nature. As shown in [Supplementary Table S10](#), S–C bonds of SO–Zn/Pc and S–C bonds of SO₃–Cd/Pc exhibit a covalent nature. Bond critical points of H₂S–Y/Pc exhibit a non-covalent nature. Other adsorption systems exhibit partially covalent nature.

Gas sensing explorations

The electrical conductivity (σ) of sensing materials changes during gas adsorption and then generate electrical signals to achieve target gas identification. The change in electrical conductivity is a critical indicator for evaluating resistive gas sensors. The decrease in the energy gap after gas adsorption causes an increase in electrical conductivity. The DOS curves of Fe/Pc, Cr/Pc and Ti/Pc before and after gas adsorption are shown in [Supplementary Fig. S11](#). For Fe/Pc and Cr/Pc, the LUMO energy level shifts slightly to the left and right, respectively, after SO and H₂S adsorption, with almost no effect on the HOMO energy level. The HOMO and LUMO energy levels of H₂S–Ti/Pc move slightly to the right compared with Ti/Pc. The shifts of these energy levels after gas adsorption causes varying degrees of changes in the energy gap. According to the results in [Supplementary Fig. S12a](#), Cr/Pc, Fe/Pc, and Ti/Pc exhibit changes of 4.12%, 1.04%, and 0.22% in ΔE_g after interacting with H₂S, resulting in decreased electrical conductivity. In contrast, an opposite trend is observed when SO adsorbs on Fe/Pc, with a significant decrement in ΔE_g (–7.93%). Therefore, it can be deduced that Fe/Pc exhibits high sensitivity for SO, followed by the Cr/Pc, Fe/Pc, and Ti/Pc for H₂S, respectively. As shown in [Supplementary Table S9](#), SO₃–Cd/Pc, SO₃–Os/Pc, SO–Zn/Pc, and H₂S–Tc/Pc complexes under an electric field exhibit more obvious changes in ΔE_g compared with the SO–Fe/Pc complex in the absence of an electric field, indicating their significantly higher sensitivity.

Fe/Pc exhibits excellent sensitivity to SO molecules, with a sensing response value of 1628.21 at room temperature. Furthermore, the Fe/Pc and Cr/Pc are sensitive to H₂S, with sensing response values of 32.22 and 1.64 at 298 K, respectively. These sensing responses are higher than the screening criteria for candidate sensing materials^[35], demonstrating their potential application as resistive gas sensors. However, Ti/Pc exhibits a lower sensing response for H₂S molecules due to the small energy gap change. As listed in [Supplementary Table S9](#), there is the highest sensing response for SO₃–Cd/Pc (8.83×10^{22}) under the electric field of 2×10^3 a.u., followed by the H₂S–Tc/Pc (3.35×10^{13} and 2.12×10^{11}) under electric fields of -4×10^3 and -6×10^3 a.u. Other adsorption systems exhibit moderate sensing response values, except for H₂S–Sc/Pc with a lower value of 0.47 (the electric field strength is 6×10^3 a.u.).

Significant changes in work function (Φ) can generate an electrical signal, which can be used to detect target gases^[53,54]. Therefore, the potential application of TM/Pc as Φ -type sensors was explored

in this study. The change in Φ of more than 10% before and after adsorption is shown in [Supplementary Fig. S12c](#), where positive and negative values represent an increase and a decrease, respectively, in work function after gas adsorption. There are three, six, four, and two promising Φ -type sensing materials for detecting H₂S, SO, SO₂, and SO₃, respectively. Among them, Cd/Pc has ultra-high gas sensitivity to SO₃ due to its significant changes in work function (36.88%).

Predicting E_{ads} and SR through the MTDL model

E_{ads} and SR are two key indicators for evaluating the potential applicability of sensing materials, as they jointly influence the adsorption–desorption equilibrium and sensing response of TM/Pc-based sensing materials. An ideal gas sensing material should balance high sensitivity with good reusability. Although E_{ads} and SR characterize different aspects of gas sensing, they both originate from the same gas–surface interaction process and therefore share complementary physicochemical information. Nevertheless, the two properties are not governed by a simple linear relationship. As shown in [Supplementary Fig. S13](#), stronger adsorption does not necessarily result in a higher sensing response, indicating that adsorption strength alone is insufficient to describe sensing performance. Consequently, E_{ads} and SR contain both shared and task-specific information, providing a strong rationale for the proposed MTDL framework, which can simultaneously exploit their common physicochemical representations while preserving the unique characteristics of each prediction task. To evaluate the effectiveness of the proposed MTDL framework, its predictive performance was systematically compared with conventional single-task machine learning models, including RF, XGBoost, GBDT, and SVM, for both classification and regression tasks.

As summarized in [Table 2](#), single-task models exhibit moderate performance in the classification task, with test-set accuracies ranging from 0.44 to 0.63. Among them, SVM achieves the highest test-set accuracy (0.63). In contrast, the MTDL framework demonstrates substantially improved classification performance, yielding an accuracy and F1-score of 0.83 and a recall of 0.88 on the independent test set. A similar advantage of MTDL is observed in the regression task for E_{ads} prediction ([Table 3](#)). While single-task models achieve reasonable predictive accuracy, with test-set R^2 values ranging from 0.62 to 0.83, the MTDL model delivers the best overall performance, achieving a test-set R^2 of 0.86 with reduced RMSE (0.46 eV) and MAE (0.35 eV). Although performance differences between cross-validation and test evaluation are still observed for MTDL, the joint optimization framework consistently outperforms single-task models on the independent test set. These results indicate that jointly learning E_{ads} and SR enables the model to better capture discriminative patterns associated with sensing performance on unseen data.

To further assess the robustness of the proposed MTDL framework, the entire modeling procedure was repeated using five independent random data splits while maintaining the same training-to-test ratio. As summarized in [Supplementary Figs. S14 and S15](#), the model consistently achieved stable predictive performance, with average five-fold cross-validation metrics of $R^2 = 0.75 \pm 0.01$, RMSE =

Table 2 Comparison of classification performance between single-task machine learning models and the MTDL framework

Model	5-fold cross-validation			Test set validation		
	Accuracy	F1-score	Recall	Accuracy	F1-score	Recall
RF	0.61	0.60	0.62	0.50	0.49	0.50
XGBoost	0.63	0.62	0.63	0.50	0.49	0.50
GBDT	0.61	0.60	0.61	0.44	0.42	0.44
SVM	0.66	0.66	0.66	0.63	0.63	0.63
MTDL	0.71	0.69	0.76	0.83	0.83	0.88

Table 3 Comparison of regression performance between single-task machine learning models and the MTDL framework

Model	5-fold cross-validation			Test set validation		
	R^2	RMSE	MAE	R^2	RMSE	MAE
RF	0.48	1.07	0.83	0.83	0.60	0.46
XGBoost	0.57	0.94	0.70	0.69	0.81	0.60
GBDT	0.51	1.00	0.76	0.66	0.84	0.51
SVM	0.58	1.02	0.77	0.62	0.88	0.76
MTDL	0.73	0.83	0.59	0.86	0.46	0.35

0.79 ± 0.02 , and $MAE = 0.57 \pm 0.01$, and average test-set metrics of $R^2 = 0.84 \pm 0.03$, $RMSE = 0.49 \pm 0.04$, and $MAE = 0.38 \pm 0.05$ (mean $\pm$ SD). For the SR classification task, the average five-fold cross-validation accuracy, F1-score, and Recall were 0.69 ± 0.03 , 0.63 ± 0.04 , and 0.69 ± 0.04 , respectively, whereas the corresponding test-set values were 0.87 ± 0.05 , 0.86 ± 0.04 , and 0.90 ± 0.03 . The consistently small standard deviations across both tasks demonstrate the robustness and reproducibility of the proposed MTDL framework under different random data partitions.

We also implemented a single-task deep learning model using the same network architecture and training pipeline as the proposed MTDL framework to ensure a fair comparison. Although the single-task model achieved slightly better regression performance (Supplementary Table S11), it requires two independent models to separately predict E_{ads} and SR. In contrast, the proposed MTDL framework jointly learns both tasks within a single model, reducing model redundancy while improving the classification performance. A systematic ablation study was further conducted to quantify the contribution of the shared backbone, Mixup augmentation, and dynamic weighting. The results demonstrate that while Mixup augmentation and dynamic weighting provide incremental gains, the multitask shared backbone is the fundamental driver of predictive performance (Supplementary Table S11).

Beyond predictive accuracy, model interpretability was further investigated using SHAP (Shapley Additive Explanations) analysis to elucidate the physicochemical factors governing the predictions of the MTDL framework (Supplementary Fig. S16). As indicated by the SHAP summary plot, the most influential features are predominantly associated with the intrinsic electronic properties of the transition metal center in TM/Pc, with the atomic radius of the transition metal (r_{TM}) ranking first, followed by the first ionization energy (I_{TM}) and the energy gap of the TM/Pc system (Gap_{TM}). This hierarchy highlights the central role of metal atomic size and electronic stability in shaping adsorption-induced electronic responses. The prominent importance of r_{TM} can be rationalized by its influence on the local coordination geometry of the metal center, which affects the accessibility of the active site and the adsorption distance between the gas molecule and the transition metal. These geometric characteristics further regulate the overlap between the metal d orbitals and the molecular orbitals of the adsorbate, thereby influencing adsorption-induced charge redistribution and the resulting electronic response^[55,56]. Charge- and electronegativity-related metal descriptors, including the Mulliken charge of the transition metal (MC_{TM}), Pauling electronegativity (N_{TM}), and electronic affinity (A_{TM}), also exhibit substantial contributions, underscoring the importance of charge distribution and electron-attracting capability of the metal center in governing gas-surface interactions. In addition, the d -band center of the corresponding pure metal surface (ϵ_d) emerges as an important descriptor, suggesting that fundamental electronic characteristics of the metal remain informative for adsorption-related trends. Beyond substrate properties, gas-phase electronic features, represented by the highest occupied molecular orbital of the gas

molecule ($HOMO_g$), contribute to the model predictions, reflecting the role of the gas electron-donating ability during adsorption. System-level descriptors of the TM/Pc material, including the dipole moment (D_{TM}) and chemical hardness (η), further influence the predictive behavior, emphasizing the relevance of polarization effects and overall electronic reactivity.

To further investigate the feature representations learned by the proposed MTDL framework, task-specific SHAP analyses were performed separately for the regression (E_{ads}) and classification (SR) heads (Supplementary Figs. S17 and S18). Although the two tasks characterize different aspects of gas sensing, they share several important descriptors. Specifically, five of the top ten ranked features, including r_{TM} , N_{ag} (average electronegativity, α_{TM} (polarizability), N_{TM} , and $HOMO_{TM}$ (highest occupied molecular orbital of TM/Pc), are common to both tasks, indicating that the shared backbone effectively captures common physicochemical representations. Meanwhile, each task also exhibits distinct high-ranking features, such as e_d and ESP_g (H/O, electrostatic potential of gas molecule) for E_{ads} prediction, and η and Gap_{TM} for SR prediction, suggesting that the task-specific heads preserve unique information relevant to their respective prediction objectives.

Collectively, these results demonstrate that the MTDL model relies on a coherent combination of transition-metal atomic properties, substrate-level electronic structure descriptors, and gas-phase frontier orbital characteristics. By integrating these descriptors, the MTDL framework simultaneously exploits the shared physicochemical representations underlying adsorption energy and gas sensing response while preserving the task-specific information associated with each prediction objective.

Conclusions

Developing advanced materials capable of efficiently detecting and removing toxic gases is essential for mitigating their environmental and health impacts, yet conventional experimental screening remains costly and time-consuming, limiting exploration across the vast chemical design space. In this work, DFT calculations were integrated with an MTDL framework to systematically investigate and predict the gas-sensing and adsorption behaviors of 28 TM/Pc materials toward four sulfur-based gases. By jointly modeling gas sensitivity and adsorption energy, the proposed MTDL framework exploits the shared physicochemical information between the two properties and achieves improved predictive performance compared with single-task models. SHAP-based feature importance analysis further reveals that the model predictions are predominantly governed by TM-centered electronic properties and system-level electronic structure descriptors, with additional contributions from gas-phase frontier orbital characteristics, highlighting the central role of electronic structure modulation and charge redistribution in adsorption-induced sensing responses. Overall, this study demonstrates that integrating DFT calculations with multitask deep learning provides a robust, interpretable, and data-driven framework for the joint prediction of

adsorption energy and gas sensing response in TM/Pc materials. The proposed framework offers mechanistic insights into the relationships between physicochemical features and sensing performance, providing practical guidance for the rational design and computational prioritization of candidate TM/Pc materials for gas detection and purification applications. Nevertheless, the present MTDL framework was developed using a relatively small dataset, which limits its generalization to completely unseen transition-metal systems. Future work will focus on substantially expanding the dataset by incorporating additional transition metals, gas molecules, and adsorption configurations, thereby improving the extrapolative capability and enabling more reliable virtual screening of novel gas-sensing materials.

Supporting Information

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The selected features and their physical interpretations (Supplementary Table S1); 28 TM atom features of TM/Pc (Supplementary Table S2); adsorption atom features of gas molecules (Supplementary Table S3); systematic features of TM/Pc (Supplementary Table S4); systematic features of gas molecules (Supplementary Table S5); sensitivity analysis α and β (Supplementary Table S6); E_{bind} and D of TM/Pc (Supplementary Table S7); E_{ads} for different adsorption systems (Supplementary Table S8); E_{ads} , percent change in E_g and SR (Supplementary Table S9); topological parameters (Supplementary Table S10); model performance and ablation study (Supplementary Table S11); infrared spectra of 3d TM/Pc (Supplementary Fig. S1); infrared spectra of 4d TM/Pc (Supplementary Fig. S2); infrared spectra of 5d TM/Pc (Supplementary Fig. S3); density of states of Pc and 3d TM/Pc (Supplementary Fig. S4); density of states of Pc and 4d TM/Pc (Supplementary Fig. S5); ESP surfaces of TM/Pc (Supplementary Fig. S6); the optimized structures and ESP (Supplementary Fig. S7); adsorption configuration under different electric fields (Supplementary Fig. S8); CDD maps under different electric fields (Supplementary Fig. S9); IGMH under different electric fields (Supplementary Fig. S10); density of states of Fe/Pc, Cr/Pc and Ti/Pc before and after gas adsorption (Supplementary Fig. S11); percent change in energy gap, sensing response and work function (Supplementary Fig. S12); relationship between E_{ads} and SR (Supplementary Fig. S13); robustness evaluation of the MTDL framework (Supplementary Figs. S14 and S15); SHAP summary plots (Supplementary Figs. S16–S18).

Author contributions

All authors contributed to the study conception and design. Yuanchao Li: Writing – original draft, DFT calculations, Funding acquisition. Ying He: Writing – original draft, Machine learning modeling. Daozhen Zhou: Data curation, Software. Hanle Chen: Validation. Yinbao Wu: Writing – review and editing. Yan Wang: Writing – review and editing. Feixiang Du: Writing – original draft, Multitask deep learning, Funding acquisition. Guohong Liu: Writing – review and editing, Data curation, Funding acquisition. Xiliang Yan: Conceptualization, Supervision, Resources, Writing – review and editing, Funding acquisition. Bing Yan: Supervision, Writing – review and editing, Funding acquisition. Yuanchao Li and Ying He contributed equally to this work. All authors read and approved the final manuscript.

Data availability

All code and data used for training models can be found at GitHub via <https://github.com/YanLabAI/TM-Pc-Sensor>.

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Declarations

Competing interests

The authors declare that they have no conflict of interest.

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