

**REVIEW**

Research Progress of Sulfide-Based Gas Sensors for the Detection of Volatile Compounds in Traditional Chinese Medicine

Jiantong Li^{1,*} and Haiqiong Huang²

¹School of Traditional Chinese Medicine, Chongqing University of Chinese Medicine, Chongqing, China

²Chongqing Chuangyuemei Intelligent Technology Co., Ltd., Chongqing, China

*Corresponding Author: Jiantong Li. Email: asahiro1018@gmail.com

Received: 13 July 2026; Accepted: 17 September 2026; Published: 12 October 2026

ABSTRACT: This paper systematically introduces the latest research results on sulfide-based gas sensors for the detection of volatile substances in traditional Chinese medicine (TCM). WS₂, SnS₂ and MoS₂ are 2D transition metal sulfides that have recently shown good results in the field of volatile organic compound (VOC) sensing, and particular attention is being paid to them. Based on relevant local and international studies, the gas-sensing mechanism, structural control strategy and application prospects of these materials in TCM volatile compound analysis have been carefully studied. Based on the above research, sulfide materials have a high specific surface area, many surface active sites, and relatively short charge transport paths; thus, they show a strong response to low-concentration VOCs at room or near-room temperatures. Improved sensing performance, such as enhanced sensitivity, altered response characteristics, reduced detection limits, etc., has been achieved through defect engineering, noble metal functionalization, heterostructure construction, and nanostructure optimisation.

KEYWORDS: Traditional Chinese medicine volatile compounds; gas sensor; electronic nose; sulfide materials

1 Introduction

Traditional Chinese Medicine is a typical example of an all-around treatment that can achieve many purposes, and has thus attracted significant attention in recent years around the world. With the rapid globalisation of TCM, at present, quality-of-life-enhancing systems for evaluation and standardised analytical methods have attracted more and more attention from scholars. Many medicinal herbs contain many kinds of VOCs that give them a particular odour, but they also have many different functions in the body, different sources around the world, different ways of being processed, and different storage requirements [1]. Previous studies have shown that the main components of VOCs in TCM are terpenes, alcohols, aldehydes, ketones, esters, and other volatile materials; together they form an odour fingerprint that can serve as an index for quality assessment, authentication, identification, and origin discrimination of herbal medicines [2].

Currently, most research on volatile compounds of traditional Chinese medicine has been conducted using traditional instruments, such as gas chromatography-mass spectrometry (GC-MS). GC-MS is an excellent, high-precision instrument, but due to the complexity of its sample preparation, high operating costs, extended analysis time, and lack of on-line monitoring, it has been widely used less frequently [3]. Gas-sensing technology, and electronic-nose (E-nose) systems are an excellent example of such technologies, they have shown rapid response speed, are easy to use and portable, have a low cost, and are suitable for

on-site measurements. Recently, E-nose platforms have been used more and more often to analyze the volatile profiles of medicinal herbs, distinguish geographical origins, classify quality and monitor storage conditions of medicinal materials [4]. In addition, the combination of sensor arrays and pattern-recognition algorithms has significantly enhanced the ability to distinguish complex odour mixtures and proposed a new strategy for intelligent quality control of traditional Chinese medicine [5].

Good working conditions for the gas sensor are generally correlated with good conditions for the sensing material. Among all the candidates, two-dimensional (2D) metal sulfides such as molybdenum disulfide (MoS_2), tungsten disulfide (WS_2) and tin disulfide (SnS_2) have gained widespread attention due to their large specific surface areas, abundant active sites, tunable electronic structures and excellent gas adsorption abilities. Sulfide-based sensing materials can often achieve high sensitivity for NH_3 , NO_2 , H_2S and other VOCs at relatively low operating temperatures or even room temperature, and are generally less sensitive than traditional metal oxide semiconductors [6]. In addition, defect engineering, heterostructure construction, morphology modulation and noble-metal functionalisation can all be used to further improve the sensing performance and, as a result, enhance sensitivity, response/recovery characteristics, selectivity and long-term stability [7]. The above attributes are suitable for the construction of high-sensitivity and selective sulfide-based gas sensors for detecting and analysing emitted volatile substances from medicinal plants.

At the same time, with the rapid development of artificial intelligence and data-driven analytical methods, new applications for sulfide-based gas sensors in TCM research have also appeared. Principal Component Analysis (PCA), Support Vector Machines (SVM), Random Forest (RF) and deep learning methods are advanced machine-learning algorithms that have been successfully applied to classify herbal species, their geographical origins and quality grades based on sensor-response patterns [4]. Sulfide-based sensor arrays and intelligent pattern recognition systems have been combined to improve the accuracy of analysis and transitioned the assessment of TCM quality from subjective sensory observation to objective, digital and intelligent methods.

Recently, research has been conducted on sulfide-based gas sensors for detecting volatile compounds in TCM, and this paper systematically introduces the progress in this area, paying particular attention to WS_2 , SnS_2 and MoS_2 -based sensing materials. Systematically explore the sensing mechanisms, including gas adsorption behaviour, surface charge transfer, defect-mediated interaction and interfacial electronic modulation, together with structural optimisation strategies, VOC detection performance and applications in electronic nose systems for TCM quality control of these materials. Finally, the current problems and future development directions are introduced to provide some references for the design and application of next-generation intelligent sensing platforms in herbal medicine analysis.

2 WS_2 -Based Gas Sensors

Tungsten disulfide (WS_2), as a typical two-dimensional transition metal dichalcogenide (TMDC), has received a lot of attention in the field of gas sensing due to its unique layered structure, tunable electronic properties, large surface-to-volume ratio, and high carrier mobility [8]. WS_2 can be used for gas sensing at a lower operating temperature than other typical metal oxide semiconductors, and sometimes at room temperature. It also has a low power consumption, structural tunability and can be used in a flexible electronic platform for VOC sensing [9]. Since the volatile components released by traditional Chinese medicines generally consist of complex VOCs, such as alcohols, ketones, terpenoids and aromatic compounds, and different medicinal materials have distinct odour profiles, WS_2 has gradually been selected as a good sensing material for analysing and detecting these volatile compounds in TCMs.

The gas-sensing performance of WS₂ is fundamentally determined by the adsorption behavior of gas molecules on the WS₂ surface and the subsequent charge-transfer-induced modulation of its electronic properties. Although a large specific surface area and abundant active sites provide more adsorption opportunities, these structural characteristics alone cannot fully explain the sensing mechanism. The interaction between gas molecules and WS₂ is strongly dependent on adsorption configurations, surface electronic states, defect structures, and interfacial charge redistribution.

Research on WS₂-based gas sensors at present mainly covers morphology control, defect engineering, heterostructure construction and E-nose integration. Donarelli et al. [8] demonstrated that edge sites and sulfur vacancies in layered WS₂ structures play important roles in gas adsorption and charge transfer. The enhanced sensing behaviour is not simply attributed to the increased number of adsorption sites. Sulfur vacancies can introduce localized electronic states near the Fermi level and generate unsaturated chemical bonds, which strengthen the interaction between gas molecules and the WS₂ surface. These defect-induced electronic states facilitate charge exchange between adsorbed molecules and the sensing layer, thereby amplifying the resistance variation during gas exposure. The authors proposed that the 2D structure is likely to increase the exposed area and shorten charge-transport paths, thus improving the response and recovery characteristics of the sensor. As shown in Fig. 1, WS₂ nanosheets are generally in a stacked layered structure and have a large number of exposed edge sites that can act as gas adsorption active centres.

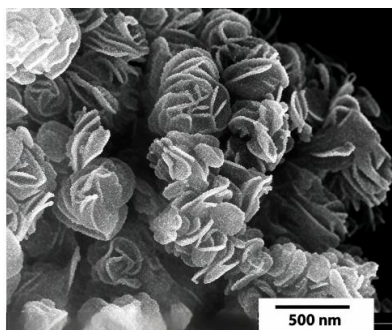


Figure 1: Morphology and gas-sensing structure of WS₂ nanosheets [9].

With the continuous progress of nanostructure preparation technology, more and more research has been carried out on the effect of WS₂ microstructures on sensing performance. Zhu et al. [9] studied layered WS₂ nanosheets and evaluated their sensing performance toward ethanol vapor. The results showed that the material responded rapidly and reversibly to low concentrations of ethanol at room temperature. The enhanced sensing performance was mainly attributed to the high density of active sites exposed at the edges of the nanosheets, which promoted ethanol adsorption and the associated charge-transfer process. Ethanol is also a representative alcohol-type volatile compound that can occur in the volatile profiles of medicinal materials and may be associated with fermentation, processing, or storage-related changes in some herbal products. Therefore, although ethanol was used as a model analyte rather than as a unique marker of TCM quality, its detection provides a useful reference for evaluating the ability of WS₂-based sensors to recognize alcohol-containing volatile components. Compared with conventional high-temperature metal oxide sensors, WS₂-based devices can operate at lower temperatures, which is beneficial for preserving thermally labile volatile compounds during TCM analysis.

Shin and others have successfully grown vertically aligned WS₂ nanosheets on Si substrates by directly chemical reacting WCl₆ vapour with sulfur-containing precursors [10]. Optimize the impact of growth temperature, carrier gas flow rate and precursor positioning systematically. The resulting vertically oriented

WS₂ nanosheets had a large specific surface area and many exposed edge sites. A relatively short multi-layer structure can also promote a high-efficiency surface charge-transfer process. Raman analysis showed that adsorbed Rhodamine 6G molecules on the surface of WS₂ generated a relatively strong Raman signal, about 9.2 times stronger than that of mechanically exfoliated monolayer WS₂. Therefore, a vertical arrangement of the molecular structure has significantly increased both the efficiency of molecular adsorption and interfacial electronic coupling. Vertically oriented nanosheets of WS₂ are relatively more exposed at the edges and have opened diffusion channels compared to the planar structures, making them more suitable for gas adsorption and transport (Fig. 2).

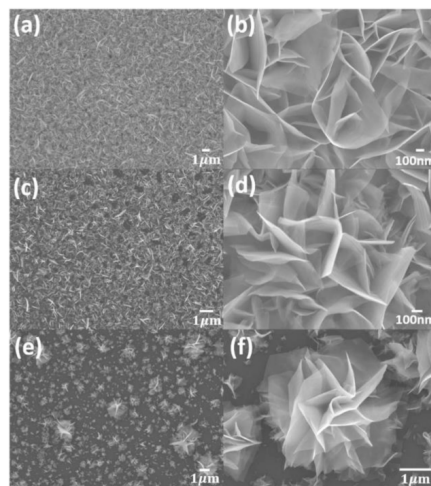


Figure 2: SEM images of vertically-oriented WS₂ nanosheets grown on a Si substrate at (a,b) 450, (c,d) 500, and (e,f) 550 °C [10].

In addition to morphology engineering, heterostructure construction and composite design have also begun to be used to improve the sensing performance of WS₂-based gas sensors. As pristine WS₂ is easily affected by humidity and lacks specific recognition of complex VOCs in a general environment, researchers have been exploring heterojunction design extensively. Dhara and others [7] have prepared a WSe₂/MoS₂ heterostructure and studied its room-temperature gas-sensing performance. Based on the above experiments, a new type of heterojunction with a different energy band structure was constructed to enhance charge carrier separation and reduce recombination. The authors have proposed that the WSe₂/MoS₂ heterojunction is a good charge-separation device, and thus has good interfacial electron transport and sensing performance.

In recent years, noble-metal functionalization and defect engineering have also emerged as important strategies for enhancing the gas-sensing performance of WS₂. Guang et al. [11] employed an *in situ* chemical reduction method to load Au nanoparticles onto WS₂ nanosheets, successfully constructing an Au/WS₂ heterostructure, and investigated its sensing response toward NH₃ at room temperature. Fig. 3 illustrates the synthesis and gas-sensing measurement of the Au/WS₂ nanocomposite-based sensor. The results indicate that, compared with pristine WS₂ (Fig. 4a), the Au-decorated nanocomposite sensor (Fig. 4b) exhibits higher response values and faster response/recovery rates for various NH₃ concentrations. With increasing Au nanoparticle loading, the sensor's response and recovery processes are further accelerated; however, at higher Au loadings, a slight decrease in sensitivity is observed. In addition, the Au/WS₂ sensor demonstrates good selectivity toward other volatile organic compounds, including formaldehyde, ethanol, benzene, and acetone. The researchers attribute the enhanced gas-sensing performance to the synergistic effects of

electronic sensitization and chemical sensitization arising from the interaction between Au nanoparticles and WS₂, which effectively promotes gas adsorption and interfacial charge transfer.

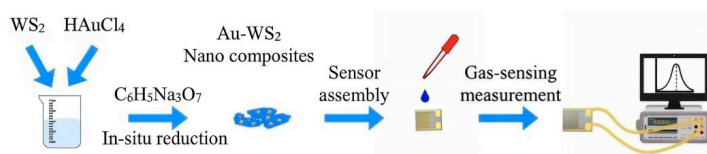


Figure 3: Schematic illustration of the synthesis and sensing measurement process of Au/WS₂ nanocomposite-based gas sensors [11].

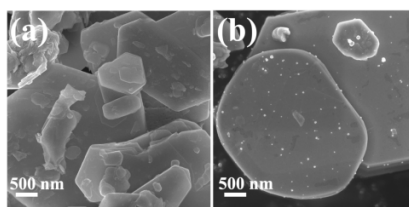


Figure 4: FESEM images of pristine WS₂ microflakes and Au/WS₂-5.6 nanocomposites; (a) FESEM image of pristine WS₂ microflowers; (b) FESEM image of Au/WS₂-5.6 nanocomposites [11].

Typically, the volatile profiles of TCMs are multi-component mixtures with low concentrations and high compositional complexity; therefore, a single sensor is not suitable for their accurate identification. As a result, sensor arrays combined with pattern recognition algorithms have been used relatively widely in the field of TCM volatile analysis. Kiani and others [2] have demonstrated that, by aggregating the responses of several sensors at different times for multiple odour samples, a system of electronic noses can be developed to evaluate the quality of medicinal plants. The three parts of a typical E-nose system are a sensor array, a signal-processing module and a pattern-recognition unit, etc. Fig. 5 is the overall process of an E-nose system. Singh et al. [12] have also used multi-sensor arrays combined with PCA and SVM algorithms to classify complex VOC mixtures. Based on the above experiments, machine-learning algorithms have shown excellent performance in enhancing the differentiation accuracy of unstable substances without introducing human error. The above ways can help to identify the plant or grass in TCM applications more quickly and accurately.

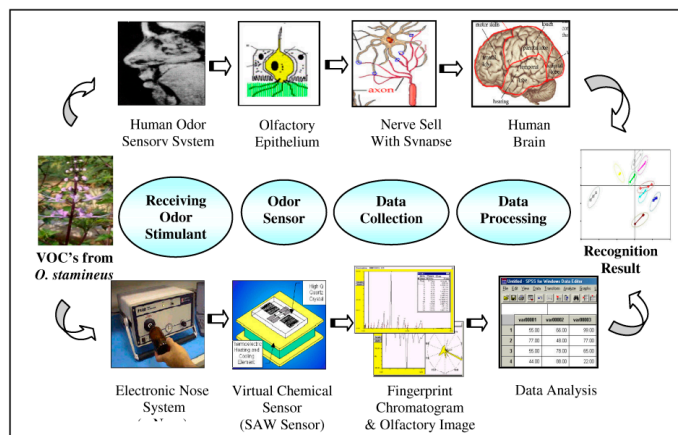


Figure 5: General workflow of an electronic nose system [13].

On the other hand, the development of flexible electronics has extended the application scope of WS_2 -based gas sensors. Kumar and others [14] have conducted an all-encompassing review of the recent development of flexible and wearable gas sensors based on 2D TMDC materials, including MoS_2 , MoSe_2 , WS_2 , WSe_2 , and SnS_2 . WS_2 has a good mechanical flexibility, high carrier mobility and many surface-active sites; thus, it has been used to build flexible sensing platforms in research. WS_2 -based flexible devices are relatively high-sensitivity detectors for many types of toxic and combustible gas at room or near-room temperatures, have good bending stability, and are also long-lasting and reliable compared with conventional rigid metal oxide sensors. TMDC-based devices are being used in electronic skin and electronic textiles by the authors as well. The flexible sensing system will also have many other uses, such as monitoring the environment and health, as well as biological volatile analysis and TCM storage supervision. A diagram of a TMDC-based flexible sensor is shown in Fig. 6.

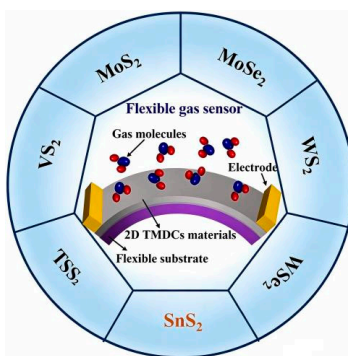


Figure 6: Schematic illustration of a flexible gas sensor based on TMDC materials [14].

WS_2 -based Gas Sensors have generally shown good support for VOC detection. Morphology engineering, heterostructure design, noble-metal functionalization and defect modulation have been employed to enhance the sensitivity, response speed and selectivity of sensors. At the same time, the combination of electronic nose technology and artificial intelligence algorithms has extended the application of WS_2 in analyzing various complex volatile substances in Traditional Chinese Medicine materials. However, most of the current studies have focused on a few standard target gases, and research on actual herbal volatile mixtures is still relatively sparse. Humidity interference, a lack of long-term stability and selectivity in a complex background environment, are also relatively serious problems that hinder practical application. Therefore, future research should focus on applying WS_2 -based sensing materials to actual systems of TCM volatile substances and developing multisensor arrays with intelligent algorithms to improve their application in the quality evaluation and quality control of TCM.

3 SnS-Based Gas Sensors

As shown in Fig. 7, the SEM images reveal the typical sheet-like morphology of the synthesized SnS. At low magnification (Fig. 7a), numerous SnS nanosheets are observed to be randomly stacked and interconnected, forming a relatively porous structure. The higher-magnification image (Fig. 7b) further reveals the layered and wrinkled characteristics of the nanosheets, with abundant exposed surfaces and edges. SnS nanosheets have been successfully prepared and investigated for gas-sensing applications, demonstrating the potential of this two-dimensional structure for gas detection [15]. When you compare it to traditional metal oxides like SnO_2 and ZnO , SnS works at lower temperatures and has higher surface activity. This is why it gets more and more attention for low-power gas-sensing uses. When we need

to detect volatile compounds that come from TCMs, the amount of VOCs that gets released from herbal materials is usually pretty low. Also, many active components in these materials break down easily when they get heated. Low-temperature responsive SnS materials thus have a lot of potential to be used in TCM electronic nose systems.

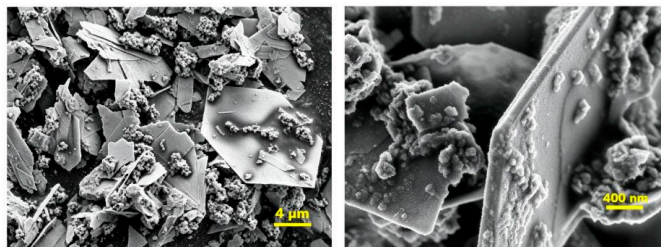


Figure 7: SEM images of SnS nanosheets: (a) low-magnification image with a scale bar of 4 μm and (b) high-magnification image with a scale bar of 400 nm [15].

At present, the main directions for the research of SnS-based gas sensors are the construction of two-dimensional structures, surface defect engineering and heterostructure design. Shan et al. [15] employed a facile chemical bath method to synthesize SnS nanosheets and investigated their ethanol-sensing properties. The results showed that the porous structure formed on the SnS nanosheets facilitated the diffusion and adsorption of ethanol molecules. As shown in Fig. 8, the sensor exhibited a substantially higher response toward 100 ppm ethanol at 160°C than toward common interfering gases such as methanol and acetone, with the response to ethanol exceeding those to the other gases by more than one order of magnitude. The authors attributed this behavior to the unsaturated sulfur atoms on the SnS surface, which provided favorable adsorption sites for ethanol, together with the two-dimensional nanosheet structure that facilitated charge transport. Ethanol is a representative alcohol-containing VOC and can be relevant to the volatile profiles of herbal materials, particularly when changes occur during fermentation, processing, or storage. From the perspective of TCM quality assessment, the ability of SnS to distinguish ethanol from other small-molecule VOCs suggests that such sensors could be incorporated into sensor arrays for monitoring changes in alcohol-related volatile profiles. However, ethanol alone cannot be regarded as a specific indicator of TCM quality because the volatile composition of medicinal materials is generally determined by multiple compounds. Its main value in current gas-sensing studies is therefore to serve as a representative analyte for evaluating the recognition capability of sensing materials toward alcohol-type VOCs.

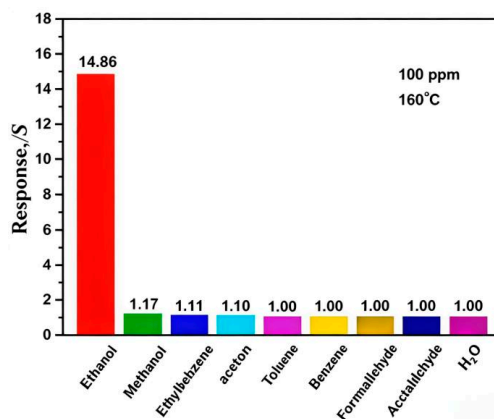


Figure 8: Responses of SnS nanosheets to various gases at 100 ppm and 160°C [15].

Besides alcohol, SnS can also be used for nitrogen oxide detection. While most of the current TCM-related nitrogen-containing volatiles have been obtained, small amounts of nitrogenous volatil can be released during herbal processing, fermentation and storage, which is interesting. Song et al. [16] construct a cross-linked SnS-nanoplate network for room-temperature NO_2 detection. Unlike dense thin films, the cross-lidized layer contains large open channels in which gases diffuse more quickly. They found that the material could respond to low concentration NO_2 at room temperature and achieve low detection limits. Their analysis indicated that large connections between connected nanoplates increased the electron depration effect, which led to more conductivity changes at the adhesion of gas adsorption. The sensor showed stable output at high humidity, which can be related to high moisture state of the TCM.

In order to improve the gas sensing performance of SnS materials, researchers have focused on connecting interfaces to build composite sensing structures. For example, formation of heterointerfaces has proved effective in controlling charge transport and surface reactions. For example, Kim et al. [17] demonstrated that air annealing could induce the formation of a SnO_2/SnS heterointerface on the material surface. Owing to the difference in energy band structures between the oxide and sulfide phases, an interfacial electron barrier was established. When target gas molecules were adsorbed onto the sensor surface, the barrier height changed accordingly, resulting in amplified conductivity variations. As a consequence, the annealed SnS sensor exhibited significantly enhanced responses toward ethanol, formaldehyde, and H_2S . The authors suggested that this improvement originated not only from morphological modifications but also from the reconstruction of the surface electronic structure induced by annealing. Similarly, Qiu et al. [18] fabricated a SnS/TiO_2 heterojunction gas sensor for room-temperature methanol detection. The introduction of the heterointerface facilitated electron transfer while effectively suppressing electron–hole recombination, thereby improving the sensing response toward low-concentration methanol. Fig. 9 presents the SEM images of the $\text{SnS}_2/\text{TiO}_2$ composite material. Since volatile ingredients, such as methanolin and ethanol, are frequently generated in the fermentation, processing and storage of some traditional Chinese medicinal materials, heterostructured sensing materials may provide opportunities to assess the quality of TCM products.

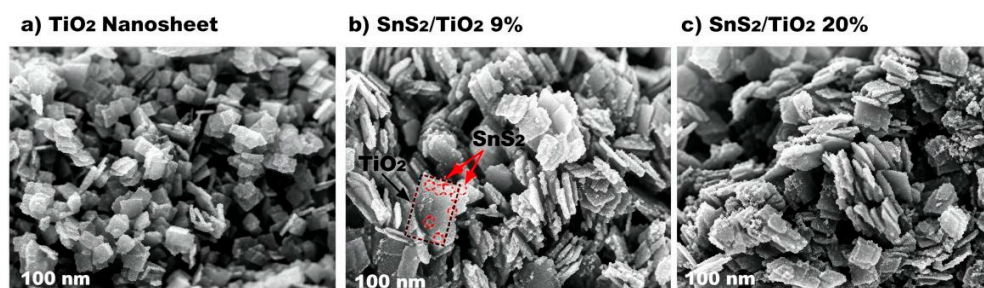


Figure 9: SEM images of (a) TiO_2 nanosheets, (b) $\text{SnS}_2/\text{TiO}_2$ composite with 9% SnS_2 , and (c) $\text{SnS}_2/\text{TiO}_2$ composite with 20% SnS_2 [19].

In addition to SnS research, SnS_2 , which has a more typical two-dimensional layered structure (Fig. 10), has also been studied. SnS_2 has a relatively high specific surface area and a larger number of active surface sites, thus being suitable for room-temperature gas sensing. Ou and others [20] reported that 2D SnS_2 nanosheets showed an obvious reversible response to NO_2 . The Two Types of Senses are Surface Adsorption and Charge Transfer. Unlike conventional metal oxides that require high-temperature chemisorption, SnS_2 can also be gas-adsorbing and gas-desorbing at a low temperature; therefore, it is suitable for flexible electronics and portable electronic nose systems. NO_2 adsorption on the surface of SnS_2 causes a redistribu-

tion of electrons in the material and thus changes in resistance. A low-temperature charge modulation mechanism is employed to enhance the low-power operation of 2D sulfide materials in gas sensing.

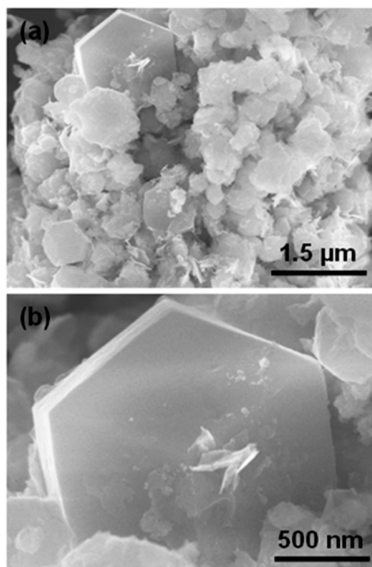


Figure 10: SEM images of pristine SnS₂ particles (a) low magnification with a 1.5 μm scale bar and (b) high magnification with a 500 nm scale bar [21].

Theoretical simulations have also provided some support for understanding the gas-sensing mechanism of SnS and SnS₂. DFT calculations have been applied to study VOC adsorption on SnS surfaces [22]. The results showed that Pt-functionalised SnS monolayers had a high adsorption energy for VOCs such as benzene and ethylene, as well as stronger electron transfer. Noble-metal functionalisation modifies the local electronic density and strengthens binding to the target molecule. Although these are still mainly computational, they provide some references for designing high-selectivity electronic nose materials.

In short, SnS-based materials can detect a large number of gases, such as NO₂, ethanol, methanol, formaldehyde and H₂S, and their development has shown a trend of two-dimensional structures, composite materials and low-temperature operation. However, most of the above studies have only considered single-component standard gases and have not comprehensively addressed the complex mixtures of VOCs in TCMs. Herbal volatile components are relatively diverse and do not have the characteristics suitable for single SnS sensors. Humidity fluctuations, background gas interference and long-term stability are also remaining problems. Table 1 lists the latest progress in SnS and SnS₂ gas-sensing performance.

Table 1: Comparison of Gas-Sensing performance of SnS- and SnS₂-based materials.

Material Type	Preparation Method	Target Gas	Operating Temperature	Response	Response/ Recovery Time	Humidity Influence	Main Advantages	Reference
SnS nanosheets	Chemical bath method	Ethanol	160°C	Response 14.86 (100 ppm ethanol)	23 s/26 s	Water molecules may compete with ethanol molecules for surface adsorption sites and influence adsorption behaviour.	Porous nanosheets facilitate ethanol diffusion and adsorption	[15]
Cross-linked SnS nanoplate network	Self-assembly	NO ₂	Room temperature	~116% (5 ppm NO ₂)	Fast response	Humidity may affect NO ₂ adsorption and surface charge-transfer processes.	Open channels and depletion-layer effect enhance gas response	[16]
SnO ₂ /SnS heterostructure	Air annealing	H ₂ S, Ethanol, Formaldehyde	Medium-low temperature	Significantly enhanced	Improved recovery	Humidity influence is related to the competitive adsorption of H ₂ O molecules and surface reaction processes.	Heterointerface strengthens electron modulation	[17]
SnS/TiO ₂ heterojunction	Composite deposition	Methanol	Room temperature	High response at low methanol concentrations	Stable	Water molecules may interfere with methanol adsorption through competitive adsorption on surface active sites.	Heterojunction promotes interfacial electron transport	[18]
2D SnS ₂ nanosheets	Liquid-phase exfoliation	NO ₂	Low temperature	High selective response	Stable reversible	High humidity may slightly decrease NO ₂ response due to competitive adsorption of H ₂ O molecules on active sites.	Surface charge-transfer effect	[20]
Pt-functionalized SnS monolayer	DFT simulation	Benzene, Ethylene, VOCs	Room temperature	Significantly enhanced adsorption energy	—	Humidity may influence VOC adsorption by competitively occupying adsorption sites.	Noble-metal modification improves VOC adsorption	[22]

4 MoS₂-Based Gas Sensors

MoS₂ has a relatively mature preparation system, a stable layered structure, and readily tunable electronic properties compared with sulfides such as WS₂ and SnS. Due to the large number of exposed edge sites and sulfur vacancies in monolayer or few-layer MoS₂, gas molecules are more prone to adsorption on the surface and participate in charge transfer. In particular, sulfur vacancies act as electron-rich centres that can regulate adsorption energy and molecular interaction strength. The adsorption-induced charge transfer modifies the carrier concentration within the atomically thin MoS₂ layer, resulting in significant conductivity changes even under low gas concentrations [8]. TCM samples generally contain low concentrations of VOCs with diverse chemical compositions. MoS₂ exhibits good performance in low-concentration gas detection and has therefore attracted considerable attention for electronic-nose systems and volatile component analysis. As a representative two-dimensional transition metal dichalcogenide, MoS₂ has been extensively investigated for gas sensing in recent years.

Early studies mainly focused on how the microstructure of MoS₂ affects its gas-sensing performance. Thang et al. [23] prepared MoS₂ nanoflower structures with different growth times using a hydrothermal method (Fig. 11) and systematically investigated their gas-sensing performance at room temperature. The results showed that, with increasing growth time, the MoS₂ nanosheets gradually assembled into larger flower-like structures. Among the investigated samples, the sample grown for 48 h exhibited the largest specific surface area and the lowest activation energy, resulting in the best gas-sensing performance. The numerous exposed edge sites and interconnected pore channels within the nanoflower structure facilitated gas diffusion and enhanced surface charge transfer, thereby improving the response to low-concentration gases.

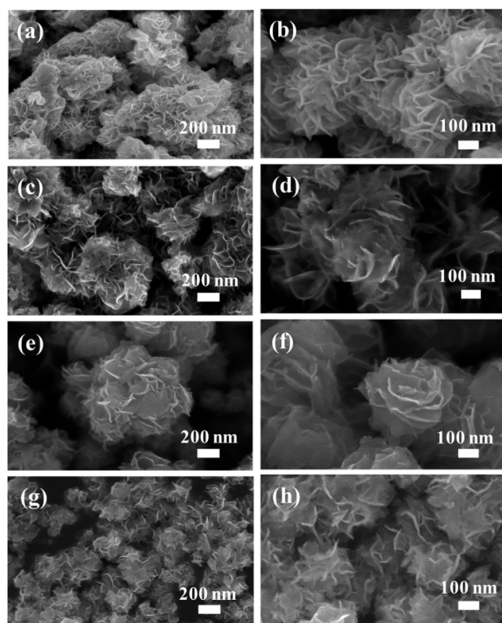


Figure 11: SEM images of MoS₂ nanoflowers synthesized at different growth times: (a,b) 24 h; (c,d) 36 h; (e,f) 48 h; (g,h) 60 h [23].

Perkins et al. [24] also observed that monolayer MoS₂ exhibited strong responses to NO₂ and NH₃. Adsorption of NO₂ resulted in a rapid decrease in conductivity, whereas NH₃ produced the opposite electrical response. This difference was mainly associated with the direction of charge transfer between the adsorbed

gas molecules and the MoS₂ surface. Because two-dimensional MoS₂ (Fig. 12) provides a short pathway for charge transport, adsorption of a relatively small number of gas molecules can induce a measurable change in electrical resistance. Conventional metal oxide sensors generally rely on thermally activated reactions involving surface oxygen species, whereas MoS₂ primarily relies on adsorption-induced surface charge modulation. This mechanism enables MoS₂-based sensors to operate effectively at room temperature.

For TCM volatile analysis, however, NO₂ should be regarded as a model analyte rather than a characteristic volatile component of TCM. Its importance mainly lies in demonstrating the relationship between molecular adsorption, charge transfer, and the resulting electrical response of MoS₂. Such mechanistic information provides a basis for understanding how MoS₂ may respond to chemically diverse volatile compounds in complex herbal samples. The low-temperature operation of MoS₂-based sensors can also reduce thermal effects on volatile compounds, making this material attractive for TCM electronic-nose applications.

Late et al. [25] developed few-layer MoS₂ thin-film gas sensors and investigated their sensing performance toward NH₃. The sensor device is capable of detecting NH₃ at the ppm level under room-temperature conditions; it also features a fast recovery speed. Reducing the layer count of MoS₂ greatly increases its specific surface area and lowers the hindrance of interlayer electron transport. These structural improvements effectively boost the sensor's gas response performance. The 2D thin-layer structure of MoS₂ offers two key advantages: it improves sensing sensitivity and cuts down device power consumption. For the detection of TCM volatiles, this low-temperature testing strategy avoids thermal damage to aromatic ingredients. As a result, it is highly applicable to the analysis of complex natural volatile systems.

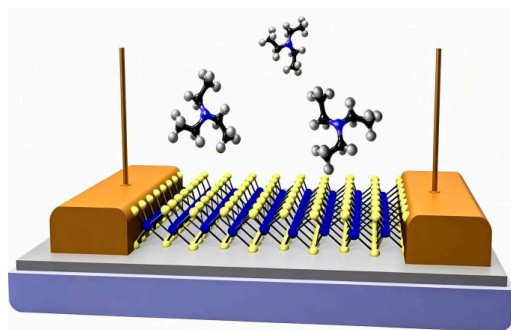


Figure 12: 2D MoS₂ model [24].

For composite structure design, Song et al. [26] developed a 3D flower-like MoS₂-ZnO micro/nanosphere array for ethanol sensing. The formation of the MoS₂-ZnO heterostructure promoted interfacial charge transfer and improved the gas-sensing performance toward ethanol. The sensor exhibited a response of 12.08 to 500 ppm ethanol at 220°C, with response and recovery times of 30 and 10 s, respectively. Compared with the pure ZnO sensor, the MoS₂-ZnO composite showed an approximately six-fold enhancement in response intensity, demonstrating the beneficial role of heterostructure construction in improving ethanol-sensing performance. Zhang et al. [27] synthesized Ni-doped, Fe-doped, and co-doped MoS₂ nanocomposites using a 1-step hydrothermal treatment and studied their room-temperature SO₂ sensing. MoS₂ sensors are faster than pure MoS₂ sensors and higher response/recovery rates for long-term experiments. Although some studies regarding sulfur-containing volatiles exist, different MoS₂ composites respond differently to alcohols, ketones and aldehydes, and give relatively stable “olfactory fingerprints”. This can be seen as a good fit to TCM aroma identification because TCM volatile components do themselves in complex mixtures, and metal-doped MoS₂ is likely to be used for analyzing complex TCM vics.

Table 2 presents the performance of the proposed MoS₂ based materials in gas sensing. According to data and literature, MoS₂ can detect VOC at low temperatures and reduces the device power required for TCM volatile components. However, most studies focus on single component standard gas and few consider high background interference in real TCM variates. Many TCM volatiles contain terpenes, esters, aldehydes and sulfur-containing compounds, which may result in cross-sensitivity which is difficult for a single MoS₂ sensor to discriminate [23].

Table 2: Comparison of gas sensing performance of different MoS₂-based materials.

Material Type	Preparation Method	Target Gas	Operating Temperature	Sensing Performance	Feature Characteristics	Reference
MoS ₂ Nanoflowers	Hydrothermal	NO ₂	Room temperature	67.4% response at 10 ppm	High specific surface area, low detection limit	[23]
Monolayer MoS ₂	Mechanical exfoliation	NO ₂ , NH ₃	Room temperature	Significant response to low-concentration gases	Pronounced charge transfer effect	[24]
Few-layer MoS ₂ Thin Film	Liquid-phase exfoliation	NH ₃	Room temperature	ppm-level detection	Low power, fast recovery	[25]
MoS ₂ /ZnO Heterostructure	Two-step synthesis	Ethanol	220°C	Response = 12.08 at 500 ppm; 30 s/10 s	Enhanced interfacial charge transfer	[26]
Metal-doped MoS ₂	Theoretical simulation	SO ₂	Room temperature	Enhanced adsorption energy	Improves selectivity	[27]

Although various modification strategies have been demonstrated to improve the sensing performance of sulfide materials, their enhancement mechanisms and practical applicability differ significantly. Therefore, a systematic comparison of these strategies in terms of fundamental mechanisms, advantages, limitations and application scenarios is summarized in Table 3.

Table 3: Comparison of modification strategies for sulfide-based gas sensors.

Modification Strategy	Fundamental Mechanism	Advantages	Limitations	Applicable Scenarios
Morphology Engineering	Modifies surface morphology and pore structure to increase exposed active sites and gas diffusion pathways.	Simple preparation; improved gas accessibility and response speed; suitable for nanosheets, nanoflowers, vertical structures.	Excessive exposure may increase humidity/environmental interference; structural stability needs improvement.	Low-concentration VOC detection; room-temperature and flexible sensors.
Defect Engineering	Introduces atomic-scale defects (e.g., sulfur vacancies) to create localized electronic states and unsaturated bonds, enhancing adsorption and charge transfer.	Boosts sensitivity and selectivity; tunes electronic structure without extra components.	Difficult to control defect concentration precisely; excess defects may cause carrier recombination and instability.	Trace gas detection; applications requiring strong molecular recognition.
Noble-Metal Functionalization	Deposits noble metal nanoparticles (e.g., Au, Pt) to provide catalytic sites and electronic sensitization via interfacial charge redistribution.	Enhances catalytic adsorption, response/recovery kinetics, and selectivity for low-concentration targets.	High cost; nanoparticle aggregation over time; complex preparation.	High-selectivity gas detection; catalytically enhanced sensing.
Heterostructure Construction	Forms interfacial electric fields and band alignment with other semiconductors to improve carrier separation and modulate charge transport.	Greatly enhances sensitivity, selectivity, and electrical response; offers additional tuning strategies.	Complex synthesis; interface stability and reproducibility are challenging.	Complex VOC mixtures; electronic nose systems; intelligent sensing platforms.
Doping Engineering	Introduces foreign elements to modify carrier concentration, adsorption energy, and surface chemistry.	Improves conductivity, selectivity, and sensing response; enables flexible electronic property control.	Hard to precisely control dopant distribution/concentration; excessive doping may damage crystal structure.	Target-specific gas detection; customized sensing materials.

5 Conclusion and Outlook

According to the above research summary, sulfide-based gas sensors are good candidates for detecting volatile ingredients in traditional Chinese medicine and have promising application prospects. However, most of the research is restricted to the laboratory, with few practical applications. TCM includes complex volatile ingredients. Traditional GC-MS analysis yields accurate results but is expensive, and testing is slow.

Two-dimensional sulfide materials MoS_2 , WS_2 , and SnS_2 can have large surface areas, strong active sites, react quickly to volatile compounds when heated, and have their own gas-sensing ability. The enhancement mechanisms of sulfide-based gas sensors vary among different modification strategies. Morphology engineering mainly improves gas diffusion and molecular accessibility, defect engineering regulates surface electronic states and adsorption behaviour, noble-metal functionalization promotes catalytic adsorption and interfacial charge transfer, while heterostructure construction improves carrier transport through interface electronic modulation. Therefore, rational selection of modification strategies according to target VOC characteristics and sensing environments is essential for developing practical TCM volatile detection systems.

The few prior studies have obvious challenges. Most experiments only test single standard gases, ignoring cross-interference caused by multiple coexisting VOCs in real TCM. Therefore, the reported experimental data may be far from actual environments. A single sensor is not able to detect complicated odors accurately, so multi-material sensor arrays are an important research area. Material doping, heterostructure construction, and composite array designs may be used later to improve recognition performance in complex gas environments.

In the future, intelligent electronic noses fused with machine learning algorithms will be able to produce individual odor fingerprints for TCM and could be used for herbal quality analysis and authenticity detection. With advances in material technology and intelligent algorithms, sulfide sensors will be miniaturized, low-power, and intelligent, and soon become more and more capable of detecting TCM in a real-world way.

Acknowledgement: The authors would like to sincerely thank their supervisors and members of the research group for their valuable guidance, constructive suggestions, and continuous support throughout the preparation of this manuscript. We also appreciate the support provided by our institution during the completion of this work.

Funding Statement: The authors received no specific funding for this study.

Author Contributions: Jiantong Li: conceptualization, writing—original draft preparation, data curation, investigation, writing—review and editing. Haiqiong Huang: writing—review and editing, supervision. All authors reviewed and approved the final version of the manuscript.

Availability of Data and Materials: Data sharing is not applicable to this article, as no datasets were generated or analyzed during the current study.

Ethics Approval: Not applicable.

Conflicts of Interest: The authors declare no conflicts of interest.

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