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Two-Dimensional Materials-Based Gas Sensors: Materials, Mechanisms, Performance and Future Directions

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Abstract: ***Two-dimensional (2D) materials are emerging candidates for next-generation gas sensors. These materials attracted pronounced attention for gas sensing applications due to their atomic-scale thickness, high surface area, and tunable electronic properties. Among 2D materials such as graphene, transition metal dichalcogenides (TMDs), MXenes, and black phosphorus enable effective gas adsorption and charge transfer, allowing sensitive and low-power detection at room temperature. This review concisely summarizes the fundamental gas sensing mechanisms in 2D materials, including chemiresistive behavior and carrier modulation, and compares recent sensor performances in terms of sensitivity, selectivity, and detection limits. Current challenges and future prospects, including defect engineering and advanced sensor architectures, are also addressed.***

Keywords: Two-dimensional materials, Gas sensors, Charge transfer mechanism

1. Introduction

The demand for sensitive and selective gas sensors has surged as society places greater emphasis on environmental protection, industrial safety, and health monitoring. With the rapid advancement of gas sensing technologies has been significantly driven by the integration of two-dimensional (2D) materials, which offer unique physicochemical properties ideal for next-generation sensor platforms [1]. Conventional gas sensing technologies, particularly metal-oxide semiconductor (MOS) sensors, such as those based on SnO_2, ZnO, WO_3, have been widely used because of their high sensitivity and simple fabrication routes [2]. However, these sensors often suffer from high operating temperatures, excessive power consumption, slow response recovery behavior, and cross-sensitivity to interfering gases [2]. The discovery of graphene and the subsequent expansion of the family of 2D materials have revitalized gas sensing research by offering atomically thin sensing platforms with extraordinary surface sensitivity [3]. These materials significantly enhance gas adsorption and charge transfer processes owing to their atomic-scale thickness, large specific surface area, and rich surface chemistry [4] [5]. Their high carrier mobility and adjustable band structures allow efficient transduction of gas surface interactions into measurable electrical signals [6]. Moreover, the mechanical flexibility of 2D materials enables integration into wearable and flexible sensor platforms [7]. Characterized by their atomic-scale thickness and high surface-to-volume ratio, 2D materials such as graphene, transition metal dichalcogenides, and MXenes exhibit exceptional electrical conductivity and chemical stability that facilitate significant gas adsorption and precise detection [8]. These materials provide an ideal platform for sensing applications due to their large specific surface area, appropriate lattice distortion, and an abundance of surface pendant bonds [4]. These structural attributes collectively enable the modulation of electrical transport properties upon gas exposure, which is fundamental for achievisor architectures [5]. Furthermore, the adaptability of these nanomaterials allows for the optimization of critical performance parameters, including room-temperature operation, rapid response kinetics, and long-term stability, which are essential for environmental monitoring and wearable applications [9]. Beyond their structural advantages, the high carrier mobility and tunable band gaps of materials like transition metal dichalcogenides and phosphorene allow for efficient charge transfer mechanisms that are critical for detecting trace concentrations of volatile organic compounds and toxic gases [6]. Figure 1 presents a schematic overview of 2D materials as gas sensors, linking their atomically thin structure to efficient charge-transfer-based sensing mechanisms**.** Gas adsorption on the 2D surface modulates carrier concentration, resulting in measurable changes in responsivity.

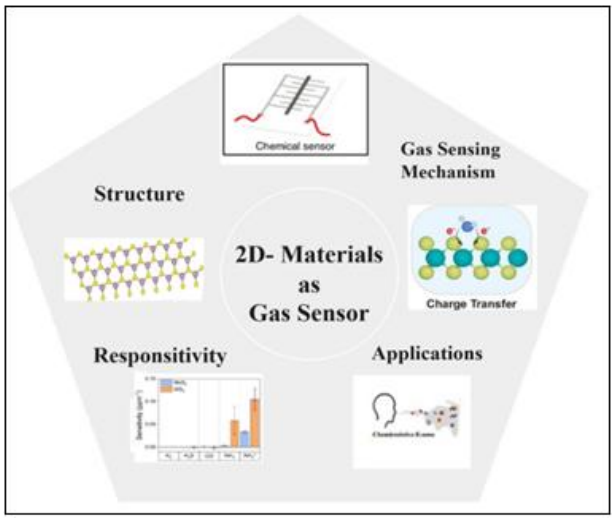

Figure 1: Schematic overview of 2D materials as gas sensors

These distinctive properties enable wide-ranging applications in environmental monitoring, healthcare, and electronic-nose systems. These structural attributes collectively enable the modulation of electrical transport properties upon gas exposure, which is fundamental for achiever architectures

[5].The ultrathin geometry means even sub-ppm levels of adsorbed molecules can significantly modulate the material's conductivity. Moreover, many 2D materials can operate at room temperature, avoiding the heating requirements of MOS sensors. For example, Lee et al. demonstrated that Ti_3C_2 MXene sheets could detect various gases at ambient conditions without external heating [10]. This high surface activity can greatly enhance gas adsorption. Reddeppa et al. further note that 2D materials often exhibit very high charge-carrier mobility and flexibility, along with large surface area and abundant defect sites [7] all advantageous for sensor function. In sum, the intrinsic properties of 2D materials – large surface area, tunable electronic structure, and rich surface chemistry – make them ideal candidates for next-generation gas sensors. The sensing mechanisms in 2D-material-based gas sensors are closely related to those of conventional chemiresistors, but with key differences. In general, a gas sensor detects an analyte via charge transfer between the target molecules and the sensing material, resulting in a measurable change in electrical conductivity.

This review systematically discusses the fundamental sensing mechanisms of 2D materials, including chemiresistive behavior, carrier concentration modulation, and mobility variation upon gas adsorption. Key material systems, device architectures, and recent performance benchmarks are critically analyzed, with emphasis on sensitivity, selectivity, response/recovery time, and detection limits. Finally, current challenges and future research directions such as defect engineering, heterostructure design, and machine-learning-assisted sensor arrays are highlighted to guide the development of highly reliable and scalable 2D gas sensing technologies.

2. 2D Materials for Gas Sensing

The specific material type and its intrinsic electronic structure play a decisive role in determining the overall sensing characteristics, as variations in surface reactivity and band gap influence the interaction strength with different gas analytes. Conventional metal oxide gas sensors have low sensitivity and require high temperatures. In contrast, 2D materials like graphene and TMDs provide high surface area and superior properties, enabling enhanced gas sensing performance through doping and heterostructures [11]. With the discovery of graphene and subsequent expansion of the family of two-dimensional (2D) materials has reignited interest in novel gas sensing platforms. Pristine graphene (a zero-gap semimetal) is extremely sensitive to adsorbates, since its conductivity shifts drastically with added charge. In the seminal work by Schedin et al., micrometer-scale graphene devices were shown to be capable of detecting adsorption events of individual gas molecules, revealing an unprecedented sensitivity that stems from graphene's atomically thin structure and ultra-low electronic noise characteristics. This work demonstrated that the adsorption or desorption of a single NO_2 molecule could alter local charge carrier concentration by discrete steps, highlighting the sensitivity of 2D materials to environmental perturbations [3]. Graphene-based sensors were among the first demonstrated (e.g. for NO_2) and have inspired many studies on doping and functionalization.[12]. Semiconducting TMDs (e.g., MoS_2, WS_2, $MoSe_2$, WSe_2) have layer-dependent bandgaps (typically 1–2 eV) and high surface activity. MoS_2 sensors, for instance, show strong responses to NO_2, NH_3 and other analytes at room temperature [13]. MXenes: These 2D transition-metal carbides/nitrides (e.g. $Ti_3C_2T_x$) are metallic or semi-metallic. MXenes can be functionalized with different surface terminations (–O, –OH, –F) and often operate natively at room temperature. Lee et al. demonstrated that a Ti_3C_2 MXene film could detect ethanol, methanol, acetone and ammonia at RT with a pronounced p-type response[14]. In general, as Bulemo et al. summarize, novel 2D sensing platforms include "graphene and its derivatives, transition metal dichalcogenides (TMDs), nitrides, bromides, MXenes, phosphorenes, and conducting metal–organic frameworks [4].

The Table 1 summarizes the major classes of 2D materials employed in gas sensing, highlighting their sensing mechanisms, performance advantages, commonly detected target gases, and key limitations.

Table 1: Summary of the major classes of 2D materials employed in gas sensing

Material	Properties	Gas sensing Mechanism	Gases Detected	Remark
Graphene and derivatives	Atomic thickness, ultra-high surface-to-volume ratio, high carrier mobility enabling large transduction of surface adsorption events [15,16]	Adsorbed gas molecules induce charge transfer or doping that changes sheet resistance (chemiresistor/FET modes) and can alter contact/depletion effects [17]	Commonly applied to oxidizing/reducing gases and VOCs such as NO2, NH3, and organic vapours [17,18]	Poor intrinsic selectivity and baseline drift; often requires functionalization/defects or heterostructures for selectivity; recovery and humidity interference are practical issues [17,18]
Transition metal dichalcogenide (TMDs) e.g., MoS_2, WS_2	Semiconducting bandgaps, abundant edge and defect sites, tunable electronic properties and surface chemistry favorable for selective adsorption[19]	Charge transfer between adsorbates and semiconductor channel changes conductivity; commonly implemented in chemiresistors and FETs; light activation and defect/ heterostructure engineering modulate responses[19]	NO2, NH3, H2, various VOCs have been demonstrated [19]	Slower recovery and stability issues under ambient conditions; selectivity and humidity sensitivity; need for defect/functionalization to reach high selectivity and speed [19]
MXenes (carbides /nitrides)	High electrical conductivity, hydrophilic surfaces with tunable surface terminations enabling strong surface interactions and rapid charge transport [20]	Surface adsorption changes conductivity; surface functional groups (–O, –OH, –F) mediate adsorption and charge exchange in	Demonstrated for NH3, NOx and VOCs [17]	Oxidation and environmental stability (air/water) limit long-term operation; termination control and scalable synthesis remain challenges[17] [20]

		chemiresistors or composite sensors [20]		
Black phosphorus (BP)	High carrier mobility and anisotropic electronic structure with reactive surface enabling strong gas interactions [17]	Adsorption induces charge transfer and large conductance changes; often used in chemiresistor/FET formats [17]	Sensitive responses to small molecules [17]	Rapid ambient oxidation and degradation require passivation; poor long-term stability limits practical use[17]
Ultrathin TMOs and 2D MOFs/COFs	Tunable chemistry, lattice distortions and abundant pendant bonds provide selective adsorption sites and catalytic surface reactions [20]	Can operate by surface oxygen ion adsorption/reaction or by mass/refractive index changes (QCM/optical) besides chemiresistive[16] [20]	Targeted detection of VOCs, NOx and other reactive gases [16] [20]	Many require controlled synthesis; some revert to bulk oxide behavior or need elevated temperatures; integration and reproducibility can be challenging [20]

3. Gas Sensing Mechanisms

The fundamental sensing mechanisms in these 2D nanomaterials primarily rely on the modulation of electrical conductance or Schottky barrier height upon the adsorption of target gas molecules, which induces charge transfer or doping effects within the semiconductor channel [21]. In general, a gas sensor detects an analyte through charge transfer between target gas molecules and the sensing material, leading to a measurable change in electrical conductivity. Gas sensing in two-dimensional (2D) materials primarily relies on charge transfer between adsorbed gas molecules and the 2D layer, which modulates carrier concentration and produces measurable changes in conductance or threshold voltage. [22][23]. Gas molecules function as electron donors or acceptors, causing charge transfer with the 2D layer and thereby altering carrier concentration and resistance [22][23]. In semiconducting TMDs such as MoS_2, this adsorption-induced doping strongly modulates electrical transport properties [3]. Furthermore, external electric fields, substrate interactions, or gate bias can regulate the magnitude and polarity of charge transfer, thereby enhancing sensitivity and selectivity in TMD-based FET sensors [3]. Gas sensing initiates with molecular adsorption via physisorption or chemisorption; weak physisorption enables reversible room-temperature sensing, whereas chemisorption leads to stronger binding and slower recovery [3,4]. Defects, edges, and surface functionalization enhance adsorption strength and charge transfer, making defect engineering and nanoparticle decoration effective strategies for improved sensitivity [2,5]. The resulting charge transfer modulates electrical signals (resistance or threshold voltage shifts) and optical responses such as photoluminescence in semiconducting TMDs [4,7]. Li S, Zhang L. et al. reported that chemiresistive gas sensors operate by monitoring resistance variations caused by gas adsorption on the sensing layer as shown in Figure 2a. These resistance changes arise from alterations in carrier concentration and mobility due to charge transfer. In 2D-materials, the sensing mechanism involves gas adsorption, surface charge transfer, and mobility modulation governed by scattering processes such as electron–phonon and ionized impurity scattering as shown in figure 2b. [24]

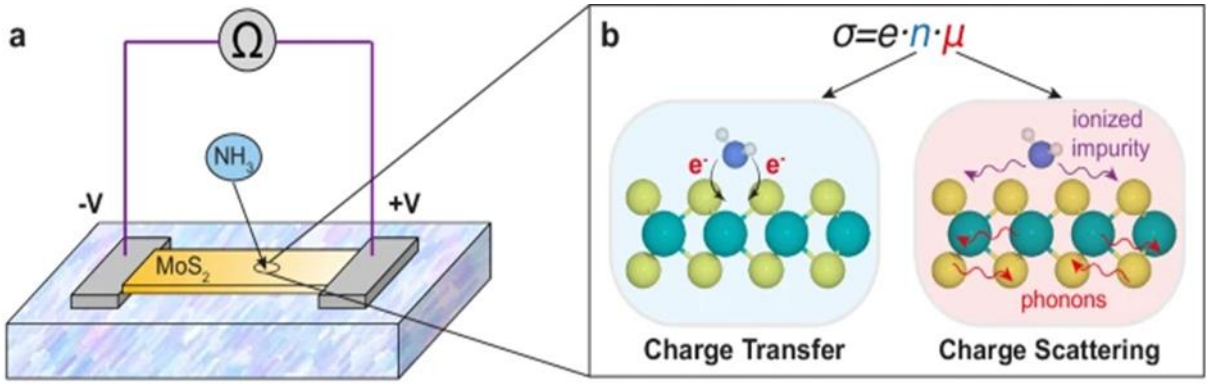

Figure 2: ***a)*** *Schematic of a 2D MoS_2–based chemiresistive NH_3 sensor.* ***b)*** *NH_3 adsorption modulates carrier concentration and mobility in 2D MoS_2, changing its resistance. Reproduced with permission* [24]. *Copyright 2024; Comput Mater*

4. Performance Comparison

Gas sensor performance is evaluated by parameters that describe magnitude, sensitivity, speed, specificity, and reliability. Key metrics are sensitivity/limit of detection, selectivity, response/recovery times, and stability/precision/accuracy, with benchmarks varying by application and material. Sensitivity is measured by exposing the sensor to known concentrations and recording the change in output; limit of detection (LOD) is established from controlled exposures and comparison to a precision reference analyzer or by statistical analysis of baseline noise and response to low concentrations [25]. Response and recovery times are routinely reported and can span seconds to minutes depending on material and operating conditions [26].

Table 2: Performance Parameters of Various 2D materials

Material / Structure	Target Gas	Concentration Tested/Temp	Response (ΔR/R or %)	Response Time	Recovery Time	LOD	Ref.
Chemically reduced graphene oxide	NH_3	200 ppm; 2800 ppm	~5.5%; 23% (ΔR/R)	–	fast (no heating)	–	[27]
MoS_2/ZnS heterostructure	NO_2	5 ppm	~7.2% (S)	–	~276 s (4.6 min)	~14 ppb	[28]
$MoSe_2$/PANI/$Ti_3C_2T_x$ (3D composite)	NH_3	1000 ppm	~6481.1 (response)	~4.7 s	~18.4 s	600 ppb	[29].
SnS_2 (15 nm flake)	NO_2	1 ppm	~4702% (response)	–	~66 s	~2 ppb	[30]
WS_2 (few-layer, p-type)	NO_2	5 ppm (25 °C)	~ *10* **%** ((R_g/R_a)	–	–	~4.7 ppb	[31]
WS_2 (few-layer, p-type)	NH_3	50 ppm (50 °C)	~7 % (R_g/R_a)	–	–	~253 ppb	[31]
$SnSe_2$ micro-flowers	NO_2	4 ppm 30°C	~5.5% (R_g/R_a)	–	–	–	[32]
Au–SnO_2 / $SnSe_2$ heterojunction	NO_2	4 ppm 80°C	~25.3% (R_g/R_a)	~156 s	~56 s	~13.7 ppb	[32]
Bilayer graphene (SAW)	NO_2 & RT	1 ppm	0.29º	–	–	68 ppb	[33]
MoS_2 film + Pt NP decoration	NH_3	2.5 ppm (RT)	Improves sensitivity ~5.6× (vs. bare)	–	–	130 ppb	[34]
MoS_2 film + Pt NP decoration	H_2S	30ppm (RT)	Improves ~4.3× (vs. bare)	–	–	5 ppb	[34]
WSe_2	NO_2	10 ppm	~1978.63%	–	–	1.25 ppb	[35]

Liu *et al.* (2022) assembled rGO with MoS_2 via a polymer, achieving sub-5 ppb LOD for both H_2S (3 ppb) and NO (5 ppb) [36]. SnS_2/MWCNT composites also achieved ppb-level NO_2 detection (5% at 25 ppb, with a theoretical ~7 ppt LOD) [37]. Yadav *et al.* employed a composite with $Ti_3C_2T_x$ MXene and polyaniline, achieving ultrahigh NH_3 response due to abundant active sites[29].These examples illustrate that 2D materials (graphene, TMDs, MXenes, etc.) and their hybrids can attain sub-ppm to ppb sensitivity in gas sensing [34,35].

5. Future Scope

Two-dimensional (2D) nanomaterials have emerged as a pivotal area of research due to their unique properties and immense potential across various applications, particularly in gas sensing [38,39]. This transformative potential stems from their exceptional physicochemical characteristics, including high surface exposure, tunable conductivity, and superior mechanical adaptability, which are crucial for detecting trace levels of various gases [40]. Moreover, the inherent quantum confinement effects and diverse elemental compositions of 2D materials allow for precise engineering of their electronic band structures and surface functionalities, thereby enabling highly selective detection of specific analytes [41]. Looking ahead, 2D materials also offer promising avenues for bionic platforms within smart technologies, bridging the gap towards advanced biomedical and healthcare applications [42] However, achieving optimal sensor performance necessitates meticulous defect engineering to enhance reactivity and selectivity, often through surface functionalization or sensor arrays integrated with machine learning algorithms [43]. This interdisciplinary approach harnesses the vast data processing capabilities of artificial intelligence to decipher complex sensing patterns, leading to more robust and accurate gas detection systems [44].

6. Conclusion

Two-dimensional materials have emerged as promising platforms for next-generation gas sensors due to their atomic thickness, high surface area, and tunable electronic properties, enabling room-temperature operation and ppb-level sensitivity. This review discussed key material systems-including graphene, TMDs, MXenes, and black phosphorus-and highlighted fundamental sensing mechanisms such as charge transfer and Schottky barrier modulation. Although significant performance improvements have been achieved through heterostructure design and surface engineering, challenges related to stability, selectivity, and scalability remain. Continued progress in material optimization and device integration will facilitate the practical deployment of 2D-material-based gas sensors in environmental, industrial, and healthcare applications.

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