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# Surface And Heterointerface Engineering Of 2D Mxenes For Gas Sensing Applications

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## ABSTRACT

Surface and heterointerface engineering of 2D MXenes have significantly propelled their potential for gas sensing applications. This study comprehensively surveys the progress made in this domain, focusing on the intricate manipulation of surface properties and heterointerfaces to enhance gas sensing performance. Firstly, the fundamental aspects of 2D MXenes, including their structure, synthesis methods, and inherent properties, are outlined. Subsequently, the principles underlying gas sensing mechanisms with 2D MXenes are elucidated, emphasizing the critical role played by surface chemistry and heterointerfaces in modulating sensing behavior. Various strategies for surface engineering, such as chemical functionalization and morphology control, are discussed in detail, highlighting their influence on gas adsorption and detection sensitivity. Additionally, the emerging field of heterointerface engineering is explored, with a focus on the creation of tailored interfaces to optimize gas-sensing properties. Recent advancements and notable achievements in gas sensing applications of engineered 2D MXenes are critically evaluated, along with existing challenges and future prospects in this rapidly evolving research area. This study serves as a comprehensive guide for researchers and practitioners interested in leveraging surface and heterointerface engineering strategies to enhance the gas sensing capabilities of 2D MXenes.

*Keywords: MXenes, Gas Sensing, Surface Engineering, Heterointerface Engineering, 2D Materials.*

## 1. INTRODUCTION

In the realm of environmental monitoring, safety protocols, and various industrial processes, gas sensing technologies play an indispensable role. These technologies rely on sophisticated devices capable of detecting the presence and concentration of specific gas molecules within a given environment. Electrochemical

sensors are a prevalent type of gas sensor. They function by utilizing a chemical reaction between the target gas and an electrolyte. This reaction generates an electrical signal whose strength is directly proportional to the gas concentration. Metal oxide semiconductor (MOS) sensors operate on a different principle. These sensors detect changes in the electrical conductivity of a

metal oxide film that occur upon exposure to gas molecules. Non-dispersive infrared sensors take a spectroscopic approach. They identify and quantify target gases by detecting the absorption of specific infrared wavelengths by the gas molecules themselves [1].

The emergence of 2D MXenes, a new class of transition metal carbides, nitrides, or carbonitrides, offers a promising avenue to overcome these limitations in gas sensing. These MXenes possess unique properties that make them strong contenders for next-generation gas sensors [2]. Their large surface areas provide ample space for gas molecules to interact, while their tunable surface chemistry allows for customization to enhance detection of specific gases. Furthermore, their inherently high electrical conductivity facilitates efficient signal transduction [3].

MXenes hold exciting potential for gas sensing applications, but their performance can be further amplified through surface and heterointerface engineering. These techniques offer precise control on a microscopic level, ultimately leading to enhanced gas sensing capabilities. One key area of improvement lies in surface area and active sites. While MXenes naturally boast a high surface area due to their 2D structure, engineering can push this even further, providing more space for gas molecules to interact with the material [4].

Selectivity, a major challenge in existing gas sensing techniques, can also be significantly improved. By strategically introducing specific functional groups through surface engineering, researchers can promote selective interactions with desired target gases. This enhances the sensor's ability to differentiate between various gases present in the environment. Sensitivity, the ability to detect low gas concentrations, is another

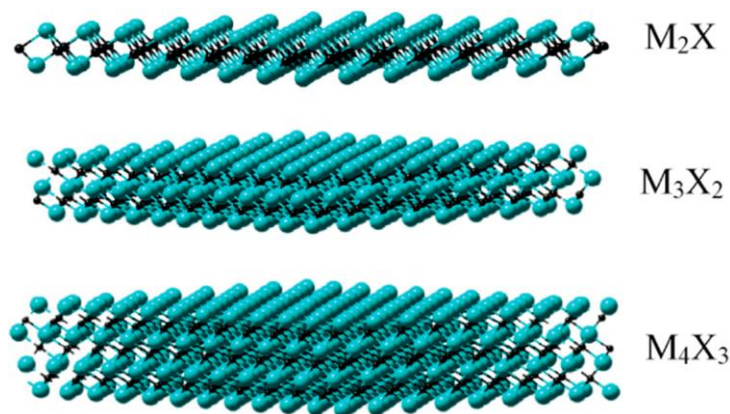
area where surface engineering plays a vital role. Optimizing the interaction between gas molecules and the MXene surface can lead to a stronger electrical response for a given gas concentration, ultimately enhancing the sensor's sensitivity [5].

MXenes are synthesized through a specific etching process that removes targeted atomic layers. This crucial step unlocks the exceptional properties that make MXenes so promising. A key advantage of 2D MXenes is their exceptionally high surface area due to their layered nature. This vast surface provides ample space for molecules to interact with the material, making them ideal for applications like gas sensing and catalysis [6]. The main objective of this study is to explore the recent advancements in engineering the surfaces and heterointerfaces of 2D MXenes for enhanced gas sensing applications. MXenes, with their inherent properties like high surface area and tunable surface chemistry, hold immense promise for gas sensing. However, by precisely manipulating their surfaces and creating interfaces with other materials, researchers can further refine their gas sensing capabilities [7].

## 2. MXenes

Transition metal carbides, nitrides, or carbonitrides, commonly referred to as 2D MXenes, represent a captivating class of nanomaterials with unique atomic structures that govern their remarkable properties. MXenes possess a layered morphology, where transition metals (e.g., titanium, zirconium) are intercalated between carbon or nitrogen atoms. This distinct arrangement, characterized by the presence of transition metals, lays the foundation for the exceptional properties exhibited by MXenes [8].

### 2.1. Structure and Properties



**Figure 1.** The initial discoveries presented three distinct configurations of 2D transition metal carbide/nitride (MXenes) by [9] available under an open access Creative Common CC BY license, at <https://www.mdpi.com/openaccess>

Due to their 2D nature and the presence of interlayer spacing between the transition metal atoms, MXenes boast an exceptionally large surface area. This extensive surface area can be visualized as a vast, sprawling landscape compared to a flat, featureless plane. The immense surface area offered by MXenes provides ample space for molecules to interact with the material, making them ideal candidates for applications such as gas sensing and catalysis. In the context of gas sensing, a larger surface area allows for a greater number of gas molecules to come into contact with the MXene, leading to a more sensitive sensor as shown in figure 1.

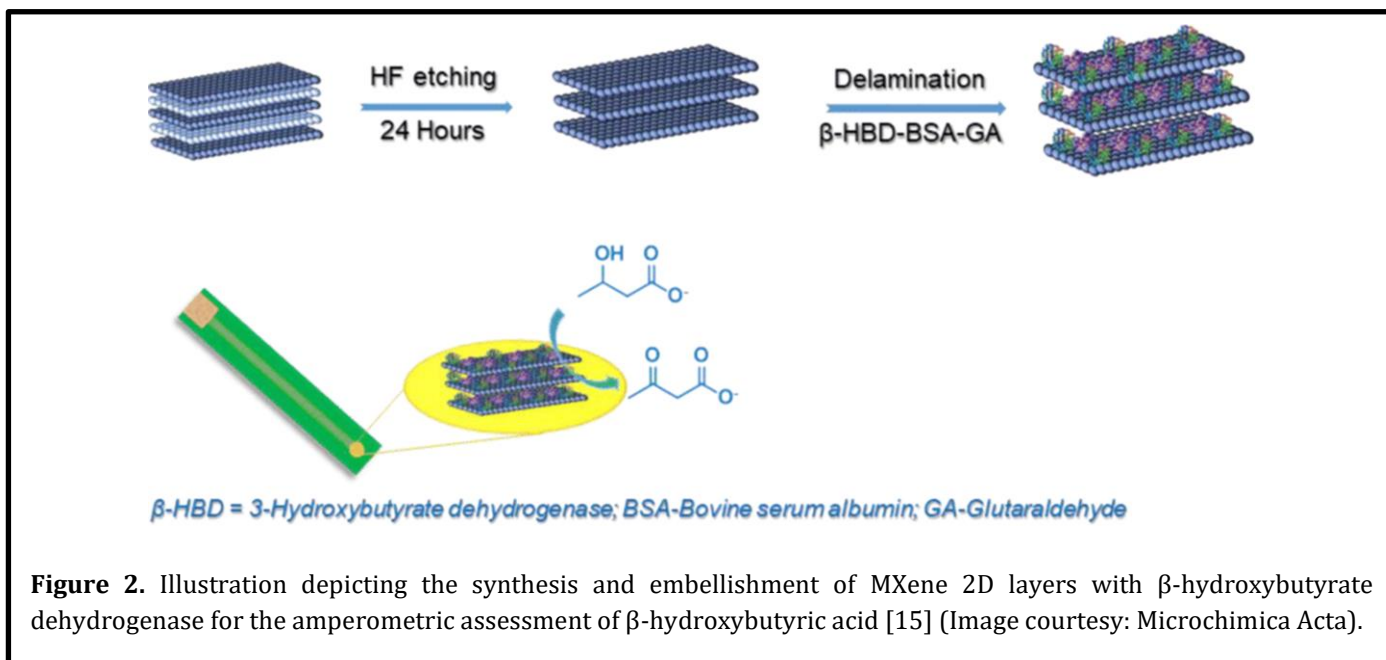
The surface of MXenes is not inert. The etching process inherently introduces functional groups, such as oxygen or hydroxyl groups, onto the surface. These groups act as unique chemical signatures, influencing how MXenes interact with their surrounding environment. However, the potential of MXenes extends beyond their inherent surface chemistry [10]. Their captivating characteristic lies in the tunability of their surface properties. By strategically introducing additional functional groups during or after the etching process, researchers can tailor MXenes for specific applications. This ability to fine-tune the surface chemistry allows for precise

control over how MXenes interact with target molecules, thereby further enhancing their effectiveness [11].

Depending on their specific composition, some MXenes exhibit excellent electrical conductivity. This property makes them valuable for applications in electronics and energy storage. In certain MXenes, the arrangement of atoms facilitates the efficient flow of electrons, akin to a highway for electrons. This characteristic makes them ideal for applications such as electrodes in batteries or transparent conductive films in electronic devices [12].

## 2.2. Synthesis Methods

The most prevalent and established method for MXene synthesis involves hydrofluoric acid (HF) etching. Here, the MAX phase precursor takes a dip in a concentrated HF solution. This acid selectively targets the A-element (often aluminum or silicon) within the MAX phase, severing the bonds that hold the layers together [13]. The transition metal carbide or nitride layers are left behind, forming the coveted MXene structure. However, achieving optimal results demands meticulous control over parameters like HF concentration, etching temperature, and duration [14]. While effective, HF's



highly corrosive and toxic nature necessitates stringent safety protocols during handling and disposal shown in figure 2.

The hazardous nature of HF has driven researchers to explore alternative etching methods. Some promising alternatives include molten salt etching, which utilizes molten fluoride salts at high temperatures for selective A-element removal. This method offers a safer route compared to HF, but might not be suitable for all MXene compositions. Another approach involves chemical etching with milder acids alongside intercalating agents (molecules inserted between MAX phase layers) to facilitate etching. This method aims to reduce reliance on HF while maintaining good control over the process. Plasma etching, another alternative, utilizes high-energy plasma for selective A-element removal. It offers precise control over etching depth but necessitates specialized equipment and might be less scalable compared to other methods.

Following the etching process, additional steps might be involved. These can include washing and centrifugation to remove residual etching agents and impurities. In

some cases, the etched MXenes might be multilayered. Techniques like sonication (using sound waves) or intercalation with specific molecules can be used to separate these layers into individual 2D sheets [16]. The selection of a synthesis method hinges on several factors, including the desired MXene composition, the safety and cost-effectiveness of the etching agent, and the required level of control over the etching process. As research progresses, the development of even more efficient and environmentally friendly methods for MXene synthesis is anticipated.

### 2.3. Gas Sensing Mechanisms

2D MXenes are revolutionizing gas sensing due to their unique properties and how they interact with gas molecules. Their high surface area provides ample space for gas molecules to land, like guests arriving at a spacious party venue. The strength of this adhesion depends on the type of gas molecule and the MXene's surface chemistry. More importantly, there can be an electron exchange between the gas molecule and the MXene, depending on the gas and the surface functional groups. This electron transfer acts as the heart of the

sensing mechanism, altering the MXene's electrical conductivity.

Imagine electron-donating gas molecules acting like generous partygoers, increasing the electron concentration in the MXene (n-type doping) and raising its conductivity. Conversely, electron-withdrawing gas molecules act like party crashers, taking away electrons (p-type doping) and lowering the conductivity. Finally, the presence of gas molecules can influence the minimum energy required to remove an electron from the MXene, impacting how it interacts with other molecules and its overall electrical properties.

By measuring these electrical changes in conductivity, current, or voltage, researchers can detect the presence and concentration of specific gases. Surface functionalization further enhances this process. By tailoring the MXene's surface chemistry, researchers can create recognition sites for specific gas molecules, leading to stronger adsorption and a more pronounced electrical response. This interplay between adsorption, charge transfer, work function change, and surface engineering paves the way for highly sensitive and selective gas sensors using 2D MXenes, with applications ranging from environmental monitoring to industrial process control.

### 2.3.1. Principles of Gas Sensing with 2D MXenes

The core of the sensing mechanism lies in the potential for electron transfer between the gas molecule and the MXene, influenced by the gas type and the MXene's surface functional groups. Imagine electron-donating gas molecules acting like generous partygoers, increasing the electron concentration in the MXene (n-type doping) and raising its conductivity. Conversely, electron-withdrawing gas molecules behave like party crashers, taking away electrons (p-type doping) and lowering the conductivity.

Beyond adsorption and charge transfer, the presence of gas molecules can also influence the minimum energy required to remove an electron from the MXene, essentially changing its work function. This impacts how the MXene interacts with other molecules and its overall electrical properties.

### 2.4. Factors Affecting Gas Sensing Performance

While 2D MXenes boast a high surface area for gas adsorption, their performance hinges on a delicate interplay of several factors as shown in table 1. Tailoring the surface chemistry with functional groups creates selective recognition sites for target gases. Porosity allows for efficient gas molecule diffusion, while intrinsic electrical conductivity translates into a stronger signal upon electron transfer. The work function, influenced by adsorbed gas, and the operating temperature further contribute to the overall sensing

**Table 1.** Illustration depicting the synthesis and embellishment of MXene 2D layers with  $\beta$ -hydroxybutyrate dehydrogenase for the amperometric assessment of  $\beta$ -hydroxybutyric acid [15] (Image courtesy: Microchimica Acta).

Factor	Description	Impact	References
Surface Area	More area for gas	Stronger signal, higher sensitivity	[17]
Surface Chemistry	Tailored for target gas	Stronger, more selective adsorption	[18]
Porosity	Pores allow gas movement	Faster response and recovery times	[19]
Conductivity	Conducts electricity	Stronger signal upon electron transfer	[20]
Work Function	Minimum energy to remove electron	Affects electrical properties, contributes to response	[21]
Temperature	Operating temperature	Optimizes adsorption or electron transfer	[22]

response. By optimizing these factors, researchers can unlock the full potential of 2D MXenes for creating highly sensitive and selective gas sensors for various applications.

### 3. Surface Modification Techniques

To push 2D MXenes towards even better gas sensing performance, researchers utilize surface modification techniques. These methods essentially tinker with the MXene surface on an atomic level. Chemical Vapor Deposition (CVD) allows for depositing a precise layer of functional groups, creating recognition sites for target gases. Diazonium salt coupling offers a similar approach by introducing specific functionalities through a reaction with the MXene's surface. Polymer grafting attaches pre-functionalized polymer chains, influencing properties like conductivity and hydrophilicity, ultimately affecting gas molecule interaction. Finally, in-situ growth of metal nanoparticles directly onto the MXene can enhance its catalytic activity and gas sensing sensitivity. By wielding this toolbox of surface modification techniques, researchers can fine-tune MXenes for exceptional gas sensing capabilities.

#### 3.1. Chemical Functionalization

By introducing specific groups onto the surface, scientists create recognition sites for target gas molecules. Imagine a perfectly sized hand on a glove - the right functional group acts like that hand, allowing only specific gas molecules (the matching key) to bind strongly (get adsorbed) to the MXene. This selectivity is crucial for distinguishing between different gases in a mixture [23].

Chemical functionalization goes beyond just recognition. It can also influence how gas molecules interact with MXenes. These functional groups can alter the electrical properties of the surface, impacting electron transfer

between the gas and the material. This electron transfer is often the core principle behind gas detection. By fine-tuning the surface chemistry, scientists can optimize this electron transfer for a stronger signal upon gas adsorption.

In essence, chemical functionalization allows researchers to transform MXenes from generic gas detectors into highly selective and sensitive sensors. By carefully crafting the surface chemistry, they can design MXenes that preferentially bind and respond to specific target gases, making them ideal for various applications like air quality monitoring or industrial process control.

#### 3.2. Physical Modification

Techniques like chemical vapor deposition or diazonium salt coupling allow scientists to introduce specific chemical groups onto the MXene surface. These groups act like recognition sites for target gas molecules. Imagine a lock and key system - the right functional group attracts the right gas molecule, leading to stronger and more selective adsorption (sticking) of the gas. This tailored surface chemistry is what makes MXenes so effective at detecting specific gases [24].

Heterointerface engineering takes things a step further. Here, scientists create interfaces by attaching other materials onto the MXene surface. These additional materials can further enhance the gas sensing properties. They might improve the conductivity of the MXene, leading to a stronger signal when gas is detected. Or, they might influence how the MXene interacts with the gas molecules, leading to even more selective and sensitive detection.

Physical modification, on the other hand, takes a different approach. Instead of changing the chemistry, it alters the physical structure of the MXene. Techniques like grinding or milling can be used to control the size

and shape of the MXene particles. This can be helpful as preprocessing before surface engineering, as exposing a larger surface area can improve the overall efficiency of the sensor. Additionally, techniques like high-pressure processing can influence the porosity (number of tiny holes) within the MXene [25]. Porosity can impact how quickly gas molecules move through the material, affecting the response and recovery times of the sensor.

So, while physical modification might not be the main act in engineering MXenes for gas sensing, it still plays a supporting role. The true stars are the surface and heterointerface engineering techniques that allow scientists to tailor the MXene's surface chemistry and interactions with target gas molecules for exceptional gas sensing performance.

#### 4. Surface Morphology Control

Techniques like etching or controlled synthesis can influence factors like the roughness, porosity, and presence of specific features on the MXene surface. A rougher surface area, for instance, can provide more sites for gas molecule adsorption, potentially leading to higher sensitivity. Similarly, well-defined pores can allow for faster diffusion of gas molecules within the MXene, improving the response and recovery times of the sensor. By strategically controlling the surface morphology, scientists can create MXenes with optimized surface area, porosity, and specific features that work in tandem with the tailored surface chemistry to achieve exceptional gas sensing performance.

##### 4.1. Surface Roughness Engineering

Surface roughness engineering enters the scene to change this. It manipulates the microscopic topography, introducing hills and valleys on the MXene surface. This seemingly minor change can significantly impact gas sensing performance [26].

A rougher surface area offers more nooks and crannies for gas molecules to land, potentially leading to a stronger signal. It's like having more real estate for gas molecules to park. Additionally, these valleys and crevices can create more favorable binding sites for specific gas molecules, crucial for selective gas sensing where only target molecules are desired. Surface roughness can even influence how gas molecules move across the MXene. By engineering specific patterns of roughness, researchers might be able to control these diffusion pathways, leading to faster sensor response times [27].

##### 4.2. Surface Defect Engineering

These defects can be vacancies, substitutions, or dislocations in the atomic arrangement of the material. While they might seem like flaws, strategically introducing or modifying these defects can offer surprising benefits for gas sensing performance [28]. The key lies in how defects can influence the interaction between MXenes and gas molecules. Defects can act as unique adsorption sites for specific gas molecules. Imagine a jigsaw puzzle with a missing piece – the right gas molecule can perfectly fit into the vacancy created by the defect, leading to strong and selective adsorption. Additionally, defects can alter the electronic properties of the MXene surface. This can influence the crucial electron transfer process that often underpins gas detection. By fine-tuning the type and concentration of defects, scientists can optimize electron transfer for a stronger overall signal upon gas adsorption [29].

Surface defect engineering offers an additional layer of control alongside established techniques like chemical functionalization. By strategically manipulating these defects, researchers can create MXenes with not only tailored surface chemistry but also optimized defect profiles for enhanced gas sensing performance. This

combined approach holds promise for pushing the boundaries of sensitivity, selectivity, and overall gas sensing capabilities of 2D MXenes [30].

## 5. Methods for Creating Heterointerfaces with 2D MXenes

One approach involves direct growth. Imagine metal nanoparticles sprouting directly on MXenes during synthesis. This intimate contact between MXene and the deposited material, achieved through techniques like hydrothermal synthesis, can lead to strong electronic coupling and improved gas sensing. Similarly, in-situ assembly involves forming another material on the MXene surface during its creation, but with more control over the interface properties by pre-mixing the precursor materials [31].

Another strategy is layer-by-layer deposition. Here, scientists meticulously build the sensor one layer at a time, alternating MXene with another material like a metal oxide. This precise approach allows for fine-tuning the composition and thickness of each layer, leading to well-defined interfaces with tailored gas sensing properties [32]. Chemical Vapor Deposition (CVD) offers another option. This versatile technique deposits a thin film of various materials onto the MXene surface, providing good control over the layer for

creating well-defined interfaces. Finally, simpler solution-based processing techniques like spin coating can be used to deposit pre-made nanoparticles onto MXenes as shown in table 2. While cost-effective, this approach offers less control over the interface properties compared to other methods.

## 6. Role of Heterointerfaces in Gas Sensing Performance

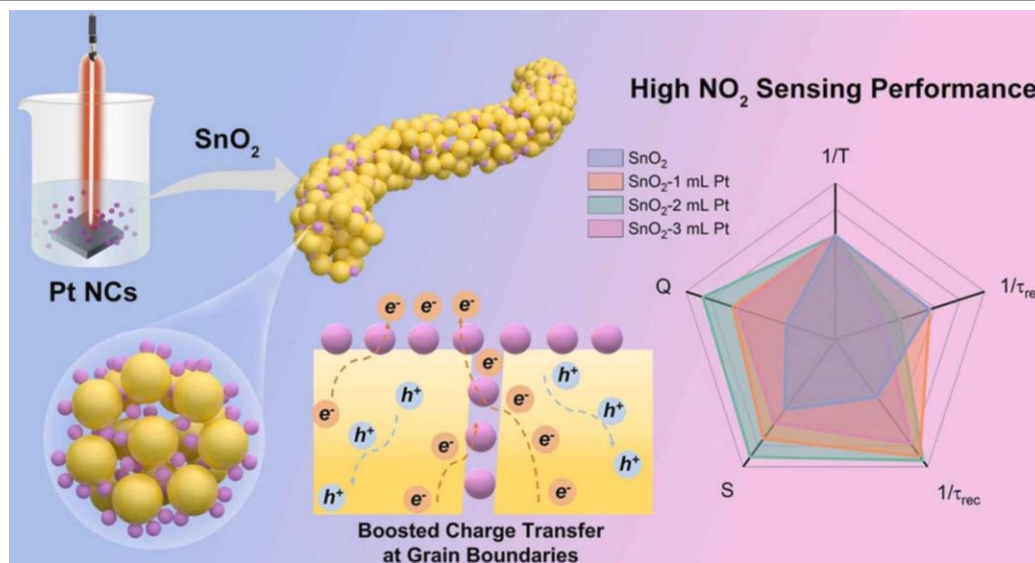
Recent research has shown that engineering heterointerfaces on 2D MXenes is a powerful strategy for enhancing their gas sensing performance. Heterointerfaces are formed when two dissimilar materials come into close contact at the atomic level. In the case of MXenes, this can involve depositing foreign atoms, molecules, or other nanomaterials onto the MXene surface. These interfaces bring several advantages to gas sensing. One key benefit is the modulation of electron transfer. The work function of the MXene and the introduced material can differ significantly as shown in figure 3. This difference creates a Schottky barrier at the interface, which affects how electrons flow within the MXene. By tailoring this modulation, researchers can improve the sensitivity of the MXene towards specific gas molecules [38].

Heterointerfaces can also increase the number of active

**Table 2.** Methods for Creating Heterointerfaces with 2D MXenes

Method	Description	Advantages	Disadvantages	References
Direct Growth	Grow materials on MXene during synthesis	Intimate interface	Less control	[33]
In-situ Assembly	Pre-mixed materials form on MXene during synthesis	Controlled growth	Complex synthesis	[34]
Layer-by-Layer Deposition	Alternating MXene & other material deposition	Precise control	Time-consuming	[35]
CVD	Thin film deposition on MXene	Good thickness control	Expensive (setup)	[36]
Solution-Based Processing	Deposit pre-made materials	Simple & cheap	Less control	[37]





**Figure 3.** Enhancing gas sensing efficiency by utilizing laser embedding to create Schottky heterointerfaces at particle boundaries within SnO<sub>2</sub> nanofibers [39] (Image courtesy: Elsevier).

sites available for gas adsorption. These sites arise due to the geometric and chemical changes at the interface compared to the pristine MXene surface. With more active sites, a greater number of gas molecules can interact with the sensor material, leading to a stronger signal. Certain heterointerfaces can even introduce catalytic properties to the MXene. These catalysts can promote specific chemical reactions between the gas molecules and the MXene surface, resulting in a more pronounced change in electrical conductivity or other sensing properties [40].

Finally, careful selection of the material introduced at the heterointerface can improve the selectivity of the MXene sensor towards specific target gases. This is achieved by tailoring the interaction between the gas molecules and the interface to be more favorable for the target gas compared to interfering species. Overall, engineering heterointerfaces provides a powerful approach for tuning the gas sensing performance of 2D MXenes. By exploiting these effects, researchers can design MXene-based sensors with high sensitivity,

selectivity, and fast response/recovery times for various gas detection applications.

### 6.1. Gas Sensing Performance of Engineered 2D MXenes

MXenes are two-dimensional materials with a large surface area relative to their volume. This provides ample space for gas molecules to adsorb, or latch onto, the MXene surface. When engineered, this surface area can be further increased by creating pores or introducing defects. Additionally, engineering can tailor the surface chemistry of MXenes, creating more active sites – specific locations on the surface that preferentially interact with target gas molecules. These factors combine to allow MXenes to interact with a high concentration of gas molecules, leading to a more significant sensor response [41].

MXenes are inherently conductive due to their metallic or semiconducting nature. When gas molecules adsorb onto the MXene surface, they can donate or withdraw electrons, causing a change in the electrical conductivity of the material. This change in conductivity is the core

principle behind how MXene gas sensors function. Engineering comes in by allowing researchers to modulate this electron transfer. By introducing heterointerfaces, where two dissimilar materials meet at the atomic level, a Schottky barrier can be formed. This barrier affects how easily electrons flow within the MXene, and by tailoring it, researchers can make the MXene more sensitive to specific gas molecules [42].

A major challenge in gas sensing is differentiating between the target gas and other gases present in the environment. Engineering MXenes can address this by allowing for improved selectivity. Here's how: By introducing functional groups onto the MXene surface during engineering, researchers can tailor the interaction between the surface and specific gas molecules. These functional groups can act like filters, allowing only the target gas molecules to bind strongly while reducing interference from other gases [43]. As mentioned earlier, careful selection of materials used to create heterointerfaces can influence how gas molecules interact with the MXene. By choosing materials that favor the target gas over others, researchers can enhance the selectivity of the sensor.

A good gas sensor needs to respond quickly to the presence of a gas and then recover back to its baseline state once the gas is removed. Engineered MXenes can be optimized for these aspects as well. Factors like porosity, surface chemistry, and the type of engineered features can all influence the response and recovery times. By optimizing these factors, researchers can create MXene sensors with fast response times and complete recovery, making them suitable for real-time gas detection applications. In conclusion, engineered 2D MXenes offer a compelling combination of high surface area, tunable electrical conductivity, and the ability to be engineered for selectivity. This makes them highly

attractive for the development of next-generation gas sensors with improved sensitivity, selectivity, response times, and recovery characteristics [44].

## 7. Comparison with Other Gas Sensing Materials

Engineered 2D MXenes offer several advantages. They can operate at room temperature, exhibit high surface area for gas adsorption, and their electrical conductivity can be readily modulated. Engineering allows for further customization, leading to improved selectivity and sensitivity. However, MXene research is still in its early stages compared to traditional materials. Challenges include developing scalable and cost-effective production methods, and improving the long-term stability of MXene-based sensors. Overall, engineered 2D MXenes show significant promise for overcoming the limitations of traditional gas sensing materials. Their unique properties and potential for improvement position them as strong contenders for revolutionizing the field [45]. Table 4.1 compares three types of gas sensing materials: Metal Oxides (MOx), Conducting Polymers (CPs), and Engineered 2D MXenes. It focuses on six key properties that are important for a gas sensor to function well.

1. **Operating Temperature:** This refers to the temperature at which the sensor material needs to operate to function effectively. Ideally, a sensor would work at room temperature (around 25°C) [46].
2. **Sensitivity:** This indicates how much the sensor's electrical signal changes in response to a gas molecule. A higher number signifies greater sensitivity.
3. **Selectivity:** This refers to the sensor's ability to distinguish between the target gas and other gases

present in the environment. A highly selective sensor only responds strongly to the target gas.

4. **Response Time:** This is the time it takes for the sensor signal to reach a stable value after exposure to a gas. A faster response time is desirable.
5. **Recovery Time:** This is the time it takes for the sensor signal to return to its baseline level after the gas is removed. A quicker recovery time allows for faster detection of subsequent gas exposures.
6. **Stability:** This refers to the sensor's ability to maintain its performance over time and under various operating conditions. A stable sensor shows consistent readings and doesn't degrade easily.

Metal Oxides (MOx) are widely used sensors but require high operating temperatures, limiting their use in portable applications. While they can be sensitive, they often struggle with selectivity and have slow response/recovery times. Conducting Polymers (CPs) offer room-temperature operation and have the potential for high sensitivity and selectivity. However, they can be unstable, particularly with regards to humidity and long-term operation. Engineered 2D MXenes show new materials show promise. They can function at room temperature, exhibit high surface area for gas interaction, and their conductivity can be tuned

for better sensitivity. Engineering allows for improved selectivity as well. However, MXenes are still under development, and challenges exist in producing them efficiently and ensuring their long-term stability [50].

## 8. Challenges and Future Directions

One key challenge is scalable and cost-effective production. Current methods are limited and expensive. Developing cheaper, large-scale production methods is crucial for commercial viability. Long-term stability under real-world conditions also needs improvement. Exposure to humidity, gases, and temperature fluctuations can affect performance over time. Optimizing sensor design and engineering for specific target gases is an ongoing effort. This involves tailoring surface chemistry, porosity, and introducing appropriate heterointerfaces to achieve desired sensitivity, selectivity, and response times. Integrating MXenes with microfabrication techniques to create miniaturized and low-power gas sensor devices is another challenge. This is essential for portable and wearable applications [51].

Despite these challenges, the future is bright for MXenes. Research is ongoing to explore new MXene compositions with tailored properties for gas sensing. This includes exploring different transition metals and functional groups for optimal performance. Developing composite materials and hybrid structures that combine

**Table 3.** Comparison of Metal Oxides (MOx), Conducting Polymers (CPs), and Engineered 2D MXenes on various properties important for gas sensing application. (1 - Low and 5 - High)

Material	Operating Temperature	Sensitivity	Selectivity	Response Time	Recovery Time	Stability	Reference
Metal Oxides (MOx)	3	1	1	3	1	1	[47]
Conducting Polymers (CPs)	4	4	4	4	4	4	[48]
Engineered 2D MXenes	2	3	3	2	3	3	[49]

MXenes with other materials like metal oxides or conducting polymers is another promising approach. This leverages the strengths of different materials to create sensors with enhanced properties.

Utilizing theoretical modeling and simulations can aid in understanding the gas sensing mechanisms in MXenes at an atomic level. This can guide the design and development of MXene-based sensors with targeted properties. Machine learning can be a powerful tool for analyzing sensor data and optimizing the design and engineering of MXenes for specific gas sensing applications. Some improvements needed. By addressing these challenges and pursuing these future directions, engineered 2D MXenes have the potential to revolutionize gas sensing. Their unique properties and the ability to tailor them through engineering make them strong contenders for developing next-generation gas sensors with superior sensitivity, selectivity, and response times. This could lead to advancements in air quality monitoring, leak detection, and medical diagnostics [52].

## 9. CONCLUSION

Engineered 2D MXenes are emerging as a revolutionary force in gas sensing due to their unique properties. Their high surface area provides ample space for gas molecules to interact, and engineering can further increase this area and tailor the surface chemistry for specific target gases. This allows MXenes to interact with a high concentration of gas molecules, leading to a stronger sensor response. A key advantage of MXenes is their inherent electrical conductivity. When gas molecules interact with the MXene surface, they can alter its conductivity. This change forms the core principle behind MXene gas sensors. Researchers can modulate this electron transfer through engineering. By introducing heterointerfaces, special junctions where

two materials meet, they can influence how easily electrons flow within the MXene. This tailored control makes the MXene more sensitive to specific gas molecules. Selectivity, a major challenge in gas sensing, can also be addressed through MXene engineering. Functional groups introduced onto the surface can act like filters, allowing only target gas molecules to bind strongly while reducing interference from others. Additionally, careful selection of materials used to create heterointerfaces can influence how gas molecules interact with the MXene, further enhancing selectivity.

Research is ongoing to explore new MXene compositions with tailored properties for gas sensing. This includes exploring different transition metals and functional groups for optimal performance. Another promising approach involves developing composite materials and hybrid structures that combine MXenes with other materials like metal oxides or conducting polymers. Machine learning can also be a powerful tool for analyzing sensor data and optimizing the design and engineering of MXenes for specific gas sensing applications. By addressing these challenges and pursuing these future directions, engineered 2D MXenes have the potential to revolutionize gas sensing.

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NA

## 11. CONFLICT OF INTEREST

The authors have declared that there is no conflict of interest.

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NA

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