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# Unveiling the potential of $Ti_3C_2T_x$ MXene for gas sensing: recent developments and future perspectives

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$Ti_3C_2T_x$  MXene, a two-dimensional transition metal carbide, has garnered significant attention as a promising material for gas sensing applications due to its exceptional properties. In this comprehensive review article, we provide an in-depth overview of the recent advancements in the field of  $Ti_3C_2T_x$ -based gas sensors. We summarize the various synthesis methods employed for  $Ti_3C_2T_x$  MXene production, including selective etching of MAX phase precursor materials and controlled annealing processes to customize its surface chemistry and properties. We thoroughly review the gas sensing properties of  $Ti_3C_2T_x$  MXene towards a wide range of gases, including volatile organic compounds (VOCs), toxic gases, and other target gases. We provide detailed insights into the gas sensing performance of  $Ti_3C_2T_x$ -based gas sensors, including sensitivity, selectivity, response and recovery times, and stability, under various temperature and gas concentration conditions. The gas sensing mechanisms involving charge transfer and surface chemisorption processes between gas molecules and the  $Ti_3C_2T_x$  MXene surface are also discussed based on experimental and theoretical studies. Furthermore, we highlight the strategies employed to enhance the gas sensing performance of  $Ti_3C_2T_x$ -based gas sensors, such as surface functionalization, doping, and hybridization with other materials. We discuss the influence of various factors, such as annealing temperature, surface modification, and device configurations, on the gas sensing properties of  $Ti_3C_2T_x$  MXene-based gas sensors. Finally, we address the challenges and future perspectives of  $Ti_3C_2T_x$ -based gas sensors, including the need for standardized testing protocols, long-term stability, and scalability of fabrication processes. Our comprehensive review aims to inspire further research efforts and promote the development of  $Ti_3C_2T_x$  MXene-based gas sensors with enhanced performance and broader applications, highlighting the promising potential of  $Ti_3C_2T_x$  MXene as a cutting-edge material for gas sensing applications.

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## 1. Introduction

In our contemporary world, marked by swift industrial growth and urban development, the significance of sensors capable of precisely identifying a wide range of hazardous gases has grown considerably. Consequently, sensitive materials, serving as pivotal elements in gas sensor technology, have garnered significant attention in ongoing research endeavors. This heightened focus is driven by their crucial roles in enhancing industrial safety, safeguarding the environment, and preserving

personal well-being.<sup>1,2</sup> At present, several materials have been investigated and established for gas sensors, such as metal oxides (MO), carbon-based materials, metal-organic frameworks (MOF), conductive polymers, rare-earth oxides, *etc.*<sup>3-12</sup> Metal oxide semiconductor (MOS) can be classified into two types, n-type (*e.g.*, ZnO, SnO<sub>2</sub>, TiO<sub>2</sub>, *etc.*) and p-type (*e.g.*, SnO, CuO, WO<sub>3</sub>, *etc.*). MO is the preferred choice for researchers as a transistor, photodetector, and gas sensor owing to its high sensitivity, high electron mobility, good transparency, low off-state current, chemical stability, compact dimensions, facile fabrication, and affordability.<sup>13-24</sup> For instance, Saini *et al.* used nanowires of Zn(II) 2,3,9,10,16,17,23,24-octakis(octyloxy)-29H,31H-phthalocyanine (ZnPcOC<sub>8</sub>) and nanoflowers of Cu(II) 2,3,9,10,16,17,23,24-octakis(octyloxy)-29H,31H-phthalocyanine (CuPcOC<sub>8</sub>) for a Cl<sub>2</sub> sensor at room temperature.<sup>25</sup> The fabricated sensor has a detection limit as low as 5 ppb and with responses as high as 715% and 550% within 10 s and 15 s by

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using simple and cost-effective self-assembly techniques. Chaloeipote *et al.* employed 3D printing technology for the synthesis of CuO, and the resulting CuO sensor demonstrated a favorable response to the detection of NO<sub>2</sub>, registering a response of 14.17% when detecting 200 ppm NO<sub>2</sub> at room temperature. Nonetheless, conventional gas sensors constructed with MO as gas-sensitive materials often attain higher response levels within

the temperature range of 200 °C to 500 °C.<sup>26</sup> This requirement for elevated temperatures not only escalates the cost of gas detection but also introduces potential safety hazards due to the elevated operating temperatures. Wang *et al.* employed KIT-6 as the rigid template for the synthesis of WO<sub>3</sub> with incorporated Au particles. The resulting Au-WO<sub>3</sub> sensor exhibited remarkable sensitivity in detecting trimethylamine, with a rapid response time of just



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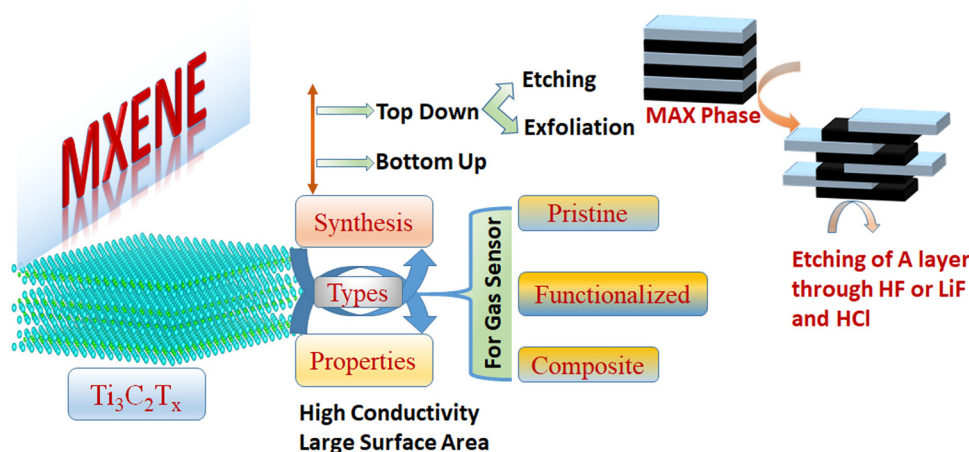


Fig. 1 Structure of the review article.

$\text{Ti}_3\text{C}_2\text{T}_x$  MXene materials can be tailored for enhanced gas-sensing performance. This review articles also summarize theoretical studies of MXene-based gas sensors using Density Functional Theory (DFT) and Molecular Dynamics (MD) simulations, which provide insights into the adsorption mechanisms and dynamic behavior of gas molecules on MXene surfaces, allowing for a comprehensive understanding of sensor performance, selectivity, and stability at the atomic level. By offering future perspectives, it goes beyond summarizing existing knowledge and sets a forward-looking agenda for researchers and engineers, helping to shape the future of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene-based gas sensing technology. This focus on recent developments and future directions positions the article as a valuable resource in the field of gas sensing, providing a more current and forward-thinking perspective compared to earlier review articles.

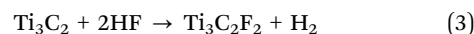
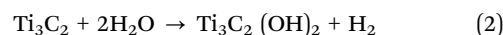
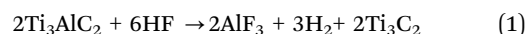
## 2. Technique for synthesis of MXenes

The techniques used to synthesize the MXene significantly affect its structure and surface functional groups, which in turn impacts the sensor's performance. The top-down etching from MAX phases is now the most widely utilized method for making MXene nanosheets. The layered structure of the MAX phase is made up of densely packed M layers and X atoms that occupy the octahedral sites and are bonded together with A atoms. In general, the M-A bond is typically thought of as a metallic bond, while the M-X bond can exhibit ionic, metallic, or covalent properties.<sup>51</sup> There are mainly two steps involved in the synthesis of MXene, *i.e.*, (1) selective etching of A layer from MAX phase and (2) delamination of MXenes from MAX phase;<sup>52</sup> both steps will discuss one by one.

### 2.1 Top-down approach

**2.1.1 Etching.** In the very first synthesis of MXene, it was suggested that an aqueous solution of hydrofluoric acid (HF) could etch the MAX phase of  $\text{Ti}_3\text{AlC}_2$ , and  $\text{Ti}_3\text{C}_2\text{T}_x$ -based MXene can be formed after selective removal of the Al layer. This

synthesis method is known as top-down synthesis and is also referred to as the main synthesis route nowadays. The etching of  $\text{Ti}_3\text{AlC}_2$  involves three reaction steps, as mentioned below



As one can see from eqn (1), during etching,  $\text{AlF}_3$  will be a byproduct that is water-insoluble; it's vital to pick the right temperature and time to avoid precipitation of  $\text{AlF}_3$ . For chemical etching, one needs to consider different reaction parameters like HF concentration, reaction time, optimum temperature, *etc.* According to the literature,  $\text{M}_{n+1}\text{AX}_n$ , with a large  $n$  number, necessitates a long etching time, a low pH value, and high etching temperature.<sup>53</sup> Therefore, a high concentration of HF is always beneficial for preferential etching of the Al layer, which can be confirmed from the structural investigation. XRD pattern exhibits a clear downshift of the (002) peak and displays the successful Al etching in  $\text{Ti}_3\text{AlC}_2$ .<sup>54</sup> Furthermore, the experimental results showed that the HF concentration can be used to rectify vacancy defects caused by the removal of surface Ti atoms.

As we know that handling HF is quite difficult, and apart from that, HF is highly corrosive in nature and not environment friendly. Furthermore, HF has a proclivity for over-corroding, resulting in defects in MXene. In 2014,  $\text{NH}_4\text{HF}_2$  was used as an etchant to avoid using toxic HF directly.<sup>55</sup> This is a significantly safer and milder alternative. In the same year, researchers also utilized LiF and HCl mixture for the etching of the Al layer in  $\text{Ti}_3\text{AlC}_2$  to form  $\text{Ti}_3\text{C}_2\text{T}_x$ .<sup>56</sup> The reaction time was 45 hours at a constant temperature of 40 °C, and the results showed that the presence of protons and fluorine ions is essential for effective etching. Later on, researchers also put more effort into refining this method by varying the feeding ratio of LiF and MAX (LiF:MAX = 5:1 or 7.5:1).<sup>57</sup> Excess LiF was found to promote Al etching and  $\text{Li}^+$  intercalation, resulting in  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene



nanosheets with identical thickness, larger size, and fewer defects. In most cases, the etching process transforms solid dense MAX into structures resembling accordions with loosely collected layers, and these formations are also referred to as multilayer MXenes. As a result, an exfoliation step is compulsory for multilayer MXenes into monolayers.

**2.1.2 Exfoliation.** Etching and delamination are the two primary processes that make up the majority of the MXene exfoliation process from the MAX phase. In the first step, a chemical etching process is used to remove the “A” layer from the middle of the MAX layers. Each MXene layer must be delaminated from the etched MAX phase in the second step. This procedure for the synthesis of MXene was carried out in a number of different ways, as shown in Fig. 2.<sup>58</sup> Each technique either incorporates HF into the MAX solution directly or introduces it indirectly through the use of LiF. The chemical connection that holds the M and X layers together can be broken apart if they are subjected to sonication, intercalants like dimethyl sulfoxide (DMSO), or ionic solutions. In any of these three scenarios, the layers are more likely to delaminate. Apart from this, LiF and HF are also favorable for non-Ti-based MXene (e.g., niobium (Nb), vanadium (V), etc.)<sup>59,60</sup>

The nanosheets of MXene were able to be exfoliated into a single layer by first inserting large organic molecules into the interlayers of the accordion-like structure and then subjecting the structure to ultrasonication or mechanical vibration.<sup>52</sup> This allowed the nanosheets to be rearranged into a single layer. The frequently used intercalants comprise  $\text{NH}_4^+$ , dimethyl sulfoxide, hydrazine, urea, and tetrabutylammonium hydroxide (TBAOH).<sup>61–63</sup> Recently, Chia *et al.* reported that by using TBAOH as the intercalant, one could exfoliate  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene from HF etching products.<sup>64</sup> After removing the A layer, expanding MAX powder that contained micron-sized flakes led to the formation of  $\text{Ti}_3\text{C}_2\text{-HF}$ , which was then delaminated into MXenes with one or more than one layers by reducing the strength of the interlayer contact with TBAOH.

## 2.2 Bottom-up approach

In addition to the top-down tactics that were discussed above, a multifunctional bottom-up approach known as chemical vapor deposition (CVD) was developed for the purpose of synthesizing high-quality and large-area MXenes. In contrast to the top-down method, which has a complex combination of groups and low controllability, the bottom-up approach has the advantage of accurately manipulating the morphology and termination groups of MXenes. The synthesis process is crucial for understanding the inherent characteristics of MXenes. Researchers reported ultrathin  $\text{Mo}_2\text{C}$ , WC, and TaC MXene crystals on Cu/Mo foil using CVD, and all of them have fewer defects with larger lateral dimensions.<sup>65</sup> The bottom-up synthesis technique of MXenes is still a big problem due to the costly equipment and tedious procedures.

In addition, if the MXene was subjected to mechanical vibration or sonication, it would contract and develop further defects. The inherent properties of 2D TMCs and TMNs have been hindered due to the chemical modification and mechanical damage that has been done to MXenes. The constituent parts of the mother 3D MAX phase have a direct influence on the structure and species of MXenes and *vice versa*. All of the MXenes that have been synthesized up to this point contain structures of the  $\text{M}_2\text{X}$ ,  $\text{M}_3\text{X}_2$ , and  $\text{M}_4\text{X}_3$  types. New synthesis methods are urgently required to improve the quality of 2D TMCs and TMNs as well as to expand the family of these materials because these MX-structured materials make up a large class of TMCs and TMNs and have a variety of fascinating properties.

The CVD production of high-quality ultrathin TMCs crystals utilizing a bilayer metal foil as a growth substrate was initially reported in 2015 by Xu *et al.*, who was also the first to reveal the technique.<sup>65</sup> The stack of Cu/Mo foils was annealed in hydrogen ( $\text{H}_2$ ) to a temperature that was higher than 1085 °C, which is the melting point of copper. Following this step, methane was injected, which led to the formation of  $\text{Mo}_2\text{C}$  crystals on the

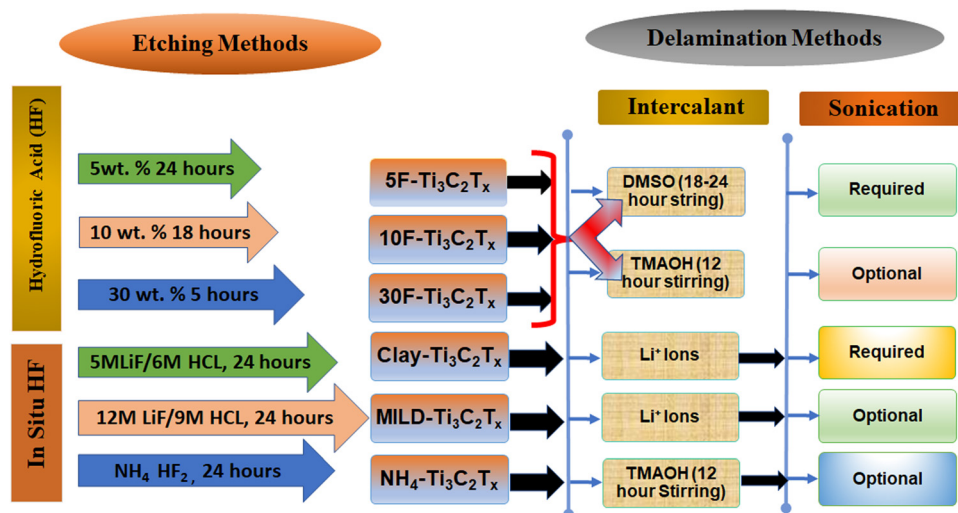


Fig. 2 Schematic diagram of the synthesis route of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene. Reproduced with permission from ref. 58 Copyright 2020. MDPI (open Access).









greater complexity compared to the conventional charge-transfer model. In the previous report on  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene based gas sensor, p-type sensing behavior was observed for ethanol, methanol, acetone, and ammonia gas at room temperature.<sup>75</sup> However, in subsequent investigations, it was observed that  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene consistently exhibited an increase in resistance when exposed to either oxidizing or reducing gases.<sup>74,76</sup> Based on the above observations, researchers proposed two possible mechanisms. (1) MXene exhibits metallic characteristics rather than semiconductor behavior, and the adsorption of gas can diminish the number of carriers while raising the channel resistance of MXene,<sup>77</sup> and (2) the expansion of MXene interlayers upon exposure to gases obstructs its electron transport in the out-of-plane direction.<sup>78</sup> Both of these mechanisms can clarify why MXenes consistently display a positive response to all gases. Though, according to Yang *et al.* report, the response signal of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene had a shift from positive to negative followed by NaOH treatment.<sup>79</sup> The change in response direction is ascribed to the rise in the O/F ratio, suggesting that surface terminations also play a noteworthy role in gas-sensing behavior. However, the fundamental mechanism behind this transformation remains unclear.

In sensors, employing hybrid structures combining MXenes and other materials, the sensor's response direction frequently hinges on the MXene's concentration within the composite. When the composite features a notably high MXenes content in conjunction with MOs, the gas response of the composite sensor aligns with that of a pure MXenes sensor, and the composite sensor exhibits significantly lower resistance compared to a pure MO sensor.<sup>80</sup> In this scenario, the presence of MOs enhances the specific surface area and facilitates the adsorption of gases.<sup>81</sup> Conversely, in situations where the MXenes content is relatively low, the gas response of the composite sensor aligns with that of the MO sensor, and the composite sensor exhibits considerably higher resistance compared to a pure MXene sensor.<sup>82</sup> In this instance, the MO take on a central role in facilitating carrier conduction during the gas-sensing process.

## 5. Why MXene for sensing applications?

The integration of sophisticated nanomaterials has ushered in a new era in the realm of sensors. When it comes to the process of signal transduction, selecting the appropriate transducer (material) is of the utmost importance. Traditional transducers suffer from the necessity of a high over-potential in the case of electrochemical sensors because of their extremely small surface area. Additionally, the target analyte's slow charge kinetics and the mass transfer constraint make it difficult for the transducer to transfer enough mass. The materials for strain sensors, instead, must preserve conductivity and mechanical strength. As a result, any viable sensor device's transducer material should have significant properties such as high surface area and high conductivity, superior mechanical strength, and a simple synthesis process. To accomplish this, a wide

range of materials, including metals, polymers, metal oxides, and carbonaceous materials, as well as their combinations, have been investigated. The race to identify the ideal combination with a high signal throughput is still ongoing despite this. In 2011, Drexel University was credited with discovering MXenes, a novel type of 2D material.<sup>30</sup> Although their primary application is in the field of energy materials, such as batteries and supercapacitors, the community of sensor researchers is showing an unusual interest in these 2D materials.<sup>83</sup> The diversity of their surface and chemical properties is directly tied to the growing application of sensor technology, which is directly related to their increasing reach. MXenes have relatively high hydrophilicity and are simple to functionalize on the surface. This is in contrast to other 2D materials like graphene, which, despite having a high conductivity, is challenging to integrate with electrode systems due to its low hydrophilicity and the fact that its sheets can be folded or re-stacked.<sup>84</sup> In addition, because of their exceptionally high conductivity, MXenes are an excellent substrate for the research and development of electrochemical sensors.<sup>33</sup> Because of their superior mechanical qualities and conductivity, MXenes provide a great conductive filler that may be used in strain and pressure sensors. It is an attractive transducing material for various sensors due to MXenes' excellent surface characteristics, metal-like conductivity, and flexibility with just the right amount of stiffness. These characteristics make MXenes suitable for electrochemical, strain bio-electrochemical, photochemical, and pressure sensors.<sup>85</sup>

## 6. Application of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene as a gas sensor

In order to make an accurate comparison of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene's application in gas sensors, the nanomaterial can be divided into three distinct classes: pure  $\text{Ti}_3\text{C}_2\text{T}_x$ , functionalized  $\text{Ti}_3\text{C}_2\text{T}_x$ , and composite  $\text{Ti}_3\text{C}_2\text{T}_x$ . This review article investigates the functionalization of  $\text{Ti}_3\text{C}_2\text{T}_x$  in terms of the alteration of functional groups and the intercalation of metal ions. Additionally, combining  $\text{Ti}_3\text{C}_2\text{T}_x$  with other materials is a successful tactic to enhance its gas-sensing performance. There are many various subgroups of materials that can be composited with  $\text{Ti}_3\text{C}_2\text{T}_x$ , including transition-metal dichalcogenides (TMDs), graphene derivatives, metal oxides, polymers, *etc.*  $\text{Ti}_3\text{C}_2\text{T}_x$  can be used to make a variety of different composites. The application in gas sensors of all three different categories of  $\text{Ti}_3\text{C}_2\text{T}_x$  will be discussed one by one.

### 6.1 Pure $\text{Ti}_3\text{C}_2\text{T}_x$ for gas sensor

After the discovery of MXene in 2011,  $\text{Ti}_3\text{C}_2\text{T}_x$  was initially used as a gas sensor, as reported by Lee *et al.*<sup>75</sup> They reported the  $\text{Ti}_3\text{C}_2\text{T}_x$ -based volatile organic compounds (VOC) gas sensor at room temperature by integrating the  $\text{Ti}_3\text{C}_2\text{T}_x$  nanosheets with solution-processed on flexible polyimide film. At ambient temperature, the  $\text{Ti}_3\text{C}_2\text{T}_x$  sensors demonstrated p-type sensing behaviour while successfully measuring methanol, ethanol,





acetone, and ammonia gas. The fabricated sensor exhibited the highest and lowest response when exposed to ammonia gas due to large adsorption energy, as shown in Fig. 4(b). Theoretically, the estimated value of the limit of detection (LOD) for acetone gas is 9.27 ppm. To detect VOC gases at parts per billion ( $10^{-9}$ ) level, Kim *et al.* proposed a  $\text{Ti}_3\text{C}_2\text{T}_x$  gas sensor with an extremely high signal-to-noise ratio (SNR).<sup>74</sup> They deposited a thin film of fully functionalized and high metallic conductivity of multi-layered  $\text{Ti}_3\text{C}_2\text{T}_x$  on a pre-printed Au electrode  $\text{SiO}_2$  substrate. The  $\text{Ti}_3\text{C}_2\text{T}_x$  gas sensor's response and SNR were compared to those of typical 2D materials (including  $\text{MoS}_2$ , black phosphorus (BP), and reduced graphene oxide (r-GO)). It was revealed that the  $\text{Ti}_3\text{C}_2\text{T}_x$  sensor's SNR was two orders of magnitude higher than that of other 2D materials because of their incredibly low noise level.  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene gas sensors showed a very low limit of detection (LOD) for VOC gases of 50–100 ppb at room temperature. A single-layer  $\text{Ti}_3\text{C}_2$ -based  $\text{NH}_3$  sensor was proposed by Wu *et al.* at ambient temperature with high selectivity [Fig. 4(c) and (d)].<sup>86</sup> Following intercalation, ultrasonic dispersion, and delamination,  $\text{Ti}_3\text{C}_2$  was coated on the ceramic tube's surface to make the gas sensor ready to detect a variety of gases, including  $\text{NO}$ ,  $\text{CH}_4$ ,  $\text{NH}_3$ ,  $\text{H}_2\text{S}$ ,  $\text{H}_2\text{O}$ , acetone ethanol, and methanol with 500 ppm concentration at room temperature. According to their research, the single-layer  $\text{Ti}_3\text{C}_2$  sensor had the highest response, which was adequately explained by first-principles calculations. Several investigations on  $\text{NH}_3$  showed that the manufactured  $\text{Ti}_3\text{C}_2$ -based sensors

have good repeatability to ammonia at room temperature, with a detection limit of 10 ppm. Additionally, utilising practical first principles, Khakbaz *et al.* thoroughly investigated the possibility of pure  $\text{Ti}_3\text{C}_2\text{T}_x$  for gas sensing.<sup>87</sup> On  $\text{Ti}_3\text{C}_2\text{T}_x$ , gas molecules such as  $\text{NH}_3$ ,  $\text{CO}$ ,  $\text{N}_2\text{O}$ ,  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{CH}_4$ ,  $\text{CO}_2$ , and  $\text{H}_2\text{S}$  were adsorbed, and the effects of various ratios of numerous functional groups were examined. The results showed that  $\text{Ti}_3\text{C}_2\text{T}_x$  is especially sensitive to  $\text{NH}_3$  relative to the other gas molecules studied, with a charge transfer of 0.098  $e$  and adsorption energy of 0.36 eV, respectively. Using first-principles analysis, Zeng *et al.* also reported that  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene is foreseen to be an encouraging sensor for  $\text{SF}_6$  decomposition characteristic components.<sup>88</sup> The adsorption strength of analytes is unevenly exhibited by different terminated  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene, and hydroxyl groups greatly enhance the adsorption strength on the  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene surface. Based on their finding they also suggested that following the adsorption of the analytes, a clear charge transfer is what primarily causes variations in  $\text{Ti}_3\text{C}_2\text{T}_x$  conductivity.

Numerous variables, including film thickness, MAX phase precursors, flake size, and degree of oxidation, have an impact on the gas sensing capabilities of pure  $\text{Ti}_3\text{C}_2\text{T}_x$ .<sup>89,90</sup> For gas (acetone, ethanol, and  $\text{NH}_3$ ) detection, Kim *et al.* also described an interfacial assembly of ultrathin  $\text{Ti}_3\text{C}_2\text{T}_x$  films.<sup>90</sup> In particular, the addition of ethyl acetate to the  $\text{Ti}_3\text{C}_2\text{T}_x$  solution promotes the production of a self-assembled layer, which had an excellent plane adhesion and stacking order. It was

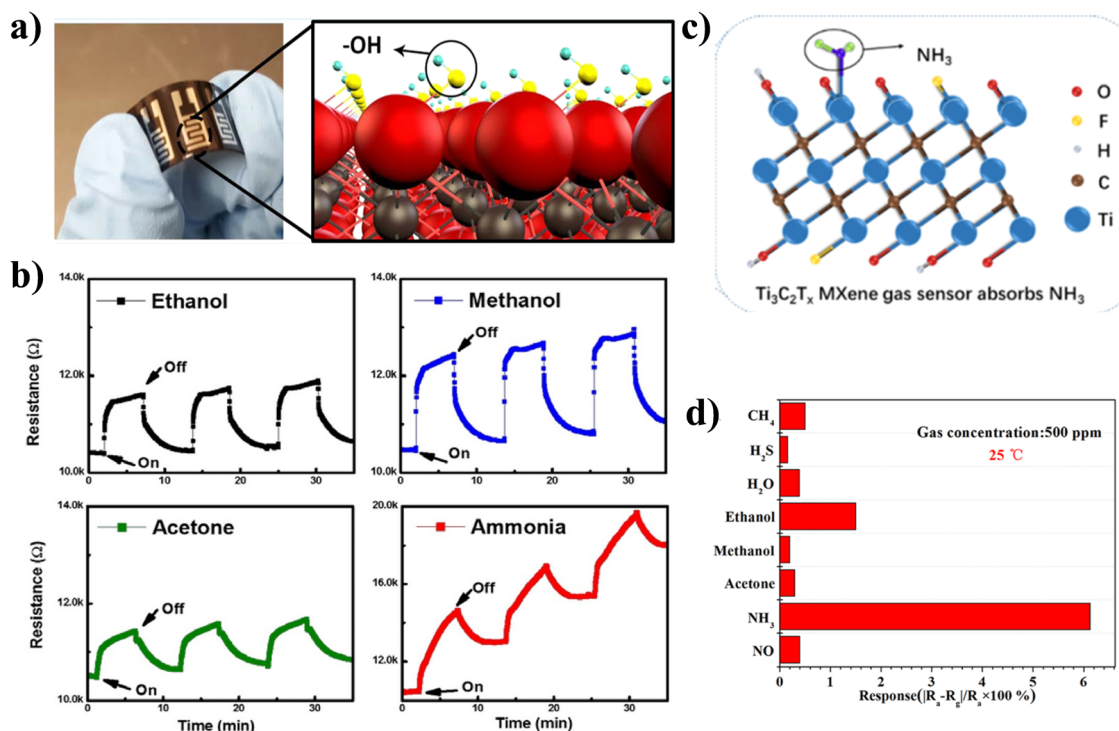


Fig. 4 (a) Schematic illustration of pure  $\text{Ti}_3\text{C}_2\text{T}_x$  VOCs, (b) results of ethanol, methanol, acetone, and ammonia gas bubbling at 100 ppm using  $\text{Ti}_3\text{C}_2\text{T}_x$  based sensor at 300 K. Reproduced with permission from ref. 75 Copyright 2017. American Chemical Society, (c) pictorial representation of absorption of  $\text{NH}_3$  on the surface of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene and, (d) room temperature response of  $\text{Ti}_3\text{C}_2$  MXene gas sensors toward 500 ppm  $\text{CH}_4$ ,  $\text{H}_2\text{S}$ ,  $\text{H}_2\text{O}$ , ethanol, methanol, acetone,  $\text{NH}_3$ , and  $\text{NO}$ . Reproduced with permission from ref. 86 Copyright 2019. American Chemical Society.



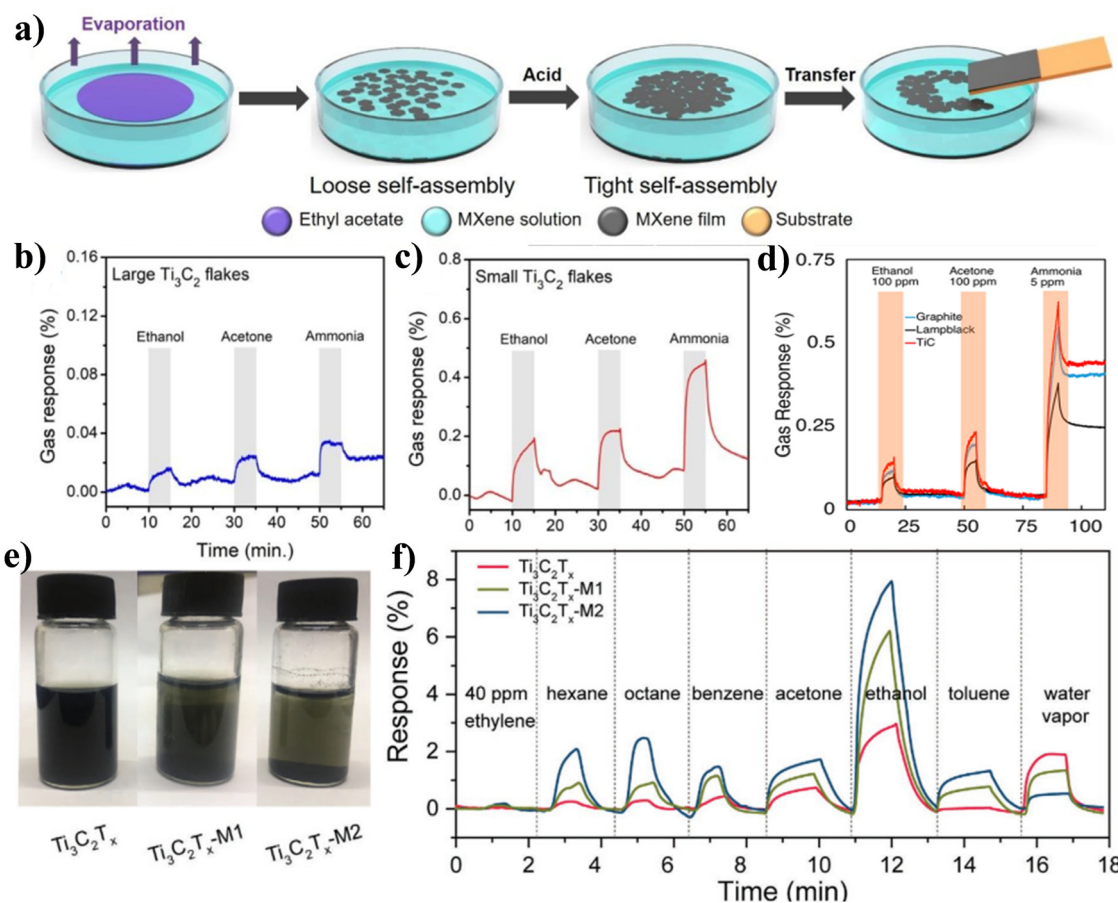


Fig. 5 (a) Schematic of the interfacial self-assembly technique for preparation of ultrathin MXene films. Gas sensing response of, (b) large  $\text{Ti}_3\text{C}_2$  flakes, (c) small  $\text{Ti}_3\text{C}_2$  flakes. Reproduced with permission from ref. 90 Copyright 2019. American Chemical Society, (d)  $\text{Ti}_3\text{C}_2\text{T}_x$ 's ability to detect gases after being made from various MAX precursors which showed different sensitivities with ethanol, acetone, and ammonia. Reproduced with permission from ref. 54 Copyright 2019. American Chemical Society, (e) photographs of pure  $\text{Ti}_3\text{C}_2\text{T}_x$ ,  $\text{Ti}_3\text{C}_2\text{T}_x\text{-M1}$ , and  $\text{Ti}_3\text{C}_2\text{T}_x\text{-M2}$  colloid solution and, (f) gas sensing performance of VOCs at 40 ppm concentration. Reproduced with permission from ref. 92 Copyright 2021. Wiley.

discovered that the self-assembly technique could improve the connectivity of small flakes, leading to minimal electrical noise in the gas sensor [Fig. 5(a) and (b)]. The gas sensor made of ultrathin  $\text{Ti}_3\text{C}_2\text{T}_x$  responded to  $\text{NH}_3$  the best, as shown in Fig. 5(c). According to research by Shuck *et al.*, the MAX phase carbon sources had an impact on the  $\text{Ti}_3\text{C}_2\text{T}_x$ 's structure and characteristics.<sup>54</sup> The three different types of  $\text{Ti}_3\text{C}_2\text{T}_x$  that were produced through etching varied in terms of chemical composition, lateral flake size, electrical conductivity, and stability. They reported that  $\text{Ti}_3\text{C}_2\text{T}_x$  made from graphite had the highest conductivity ( $4400 \text{ S cm}^{-1}$ ) and was the most stable (time constant, 10.1 days), whereas MXene made from TiC had a similar conductivity ( $3480 \text{ S cm}^{-1}$ ) but had the lowermost colloidal stability (4.8 days) as well as the lowest chemical stability (5.1 days). The most responsive to gases and with good selectivity to  $\text{NH}_3$  was the TiC-produced  $\text{Ti}_3\text{C}_2\text{T}_x$ , as shown in Fig. 5(d). In spite of this,  $\text{Ti}_3\text{C}_2\text{T}_x$  has not made significant progress in the field of gas sensors due to the fact that it is easily oxidized and has a tendency to be unstable. Chae *et al.* looked into the key variables (including water molecules, temperature, and solvents) controlling the oxidation of  $\text{Ti}_3\text{C}_2\text{T}_x$

in order to get around this constraint. They proposed that low temperature and ethanol solvent can help in maintaining the intrinsic properties of prepared  $\text{Ti}_3\text{C}_2\text{T}_x$ .<sup>91</sup> For the purpose of detecting VOCs at room temperature, Liu *et al.* recently proposed termination-modified  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene ( $\text{Ti}_3\text{C}_2\text{T}_x\text{-M}$ ) through alkali pre-treatment and trimethylacetic anhydride functionalization [photograph is shown in Fig. 5(e)].<sup>92</sup> In comparison to its unprepared counterpart, the  $\text{Ti}_3\text{C}_2\text{T}_x$  sensor showed a fivefold increase in response to ethanol with a 29% reduction in response to water vapor followed by the spray coating methods, as shown in Fig. 5(f).

In summary, one notable advantage of pristine  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene-based gas sensors is their exceptional sensitivity and rapid response to a wide range of gases. These sensors exhibit high surface area, enabling effective gas adsorption, and their 2D layered structure provides numerous active sites for gas molecules to interact with, resulting in enhanced detection capabilities. Additionally, MXene-based sensors often possess excellent electrical conductivity, facilitating quick and precise signal readouts. These properties make them highly versatile for gas sensing applications, ranging from environmental



monitoring to industrial safety, where the ability to detect and respond to diverse gas species swiftly and accurately is of paramount importance. However, one significant drawback of pristine  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene-based gas sensors is their limited selectivity when detecting multiple gases simultaneously. The inherent reactivity of MXene materials can lead to cross-sensitivity issues, making it challenging to distinguish between different gas species accurately. The MXene's hydrophilic nature can lead to water absorption, which interferes with gas sensing performance and reduces sensitivity. To overcome this limitation, researchers have been exploring strategies such as surface functionalization and composite material design, which we will discuss one by one in next section. Surface modification with specific functional groups or the incorporation of other nanomaterials can enhance the selectivity of MXene-based sensors by tailoring their chemical affinity to target gases. These advancements in MXene-based gas sensors hold promise for enhancing their practical utility in real-world applications.

## 6.2 Functionalized $\text{Ti}_3\text{C}_2\text{T}_x$ for gas sensor

Even though  $\text{Ti}_3\text{C}_2\text{T}_x$  has metallic properties when it is pure, its electronic properties can be changed by functionalization and become semiconducting. The functionalization can be done through metal ion intercalation,<sup>93</sup> sulphur doping,<sup>94</sup> oxidation,<sup>95</sup> noble metal modification,<sup>96</sup> and functional group modification.<sup>97,98</sup> Researchers have started to pay more attention to functionalization because it can improve the adsorption effect of  $\text{Ti}_3\text{C}_2\text{T}_x$ , which is favorable for gas sensing applications. Metal ion intercalation was studied by Koh *et al.* as part of their investigation into how gas-induced interlayer swelling

of  $\text{Ti}_3\text{C}_2\text{T}_x$  influences the performance of gas sensing.<sup>93</sup> When NaOH was utilized as the ionic intercalating agent, the *in situ* X-ray diffraction (XRD) experiments demonstrated a significant relationship between the gas response and the interlayer transport caused by the interlayer ions as shown in Fig. 6(a). The highest level of sensitivity was reported in  $\text{Ti}_3\text{C}_2\text{T}_x$  after treatment with  $0.3 \text{ mmol L}^{-1}$  NaOH, and the highest response was achieved for ethanol, as shown in Fig. 6(b). Similar to this, Yang *et al.* enhanced the gas sensing performances of the organ-like  $\text{Ti}_3\text{C}_2\text{T}_x$  by  $-\text{OH}$  functional alteration and alkaline metal ion (Na) intercalation.<sup>79</sup> The sensing components were uniformly coated on the  $\text{Al}_2\text{O}_3$  ceramic substrate by drop-coating process to create the pristine  $\text{Ti}_3\text{C}_2\text{T}_x$  and alkalized  $\text{Ti}_3\text{C}_2\text{T}_x$  gas sensors to study the alkalized  $\text{Ti}_3\text{C}_2\text{T}_x$ 's gas sensing performance and the schematic is shown in Fig. 6(c). It was discovered that the alkalized  $\text{Ti}_3\text{C}_2\text{T}_x$  exhibited the opposite tendency to the pristine  $\text{Ti}_3\text{C}_2\text{T}_x$ , whose resistance rose with the concentration of  $\text{NH}_3$ . The highest response with alkalized  $\text{Ti}_3\text{C}_2\text{T}_x$  was achieved in  $\text{NH}_3$  gas (around 28.7% more than pristine  $\text{Ti}_3\text{C}_2\text{T}_x$ ) and the selectivity also enhanced with alkalized  $\text{Ti}_3\text{C}_2\text{T}_x$  (ethanol, acetaldehyde, formaldehyde, methanol, acetone, methane, and  $\text{NO}_2$ ) as shown in Fig. 6(d).

The inherently metallic  $\text{Ti}_3\text{C}_2\text{T}_x$  was functionalized with oxygen by Pazniak *et al.* to increase gas sensitivity. Fig. 7(a)–(g)<sup>95</sup> shows that  $\text{Ti}_3\text{C}_2\text{T}_x$  had been partially oxidized kept its conductivity at the optimum annealing temperature of  $350^\circ\text{C}$ , and the  $\text{TiO}_2$  formed during oxidation improved its detection capacities to gases at concentrations as low as  $10^{-6}$ . The partially oxidized multisensor array-based  $\text{Ti}_3\text{C}_2\text{T}_x$  demonstrated strong response values and selectivity for acetone. Recently, Yao *et al.* also demonstrated a partially oxidized  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene-based sensor which

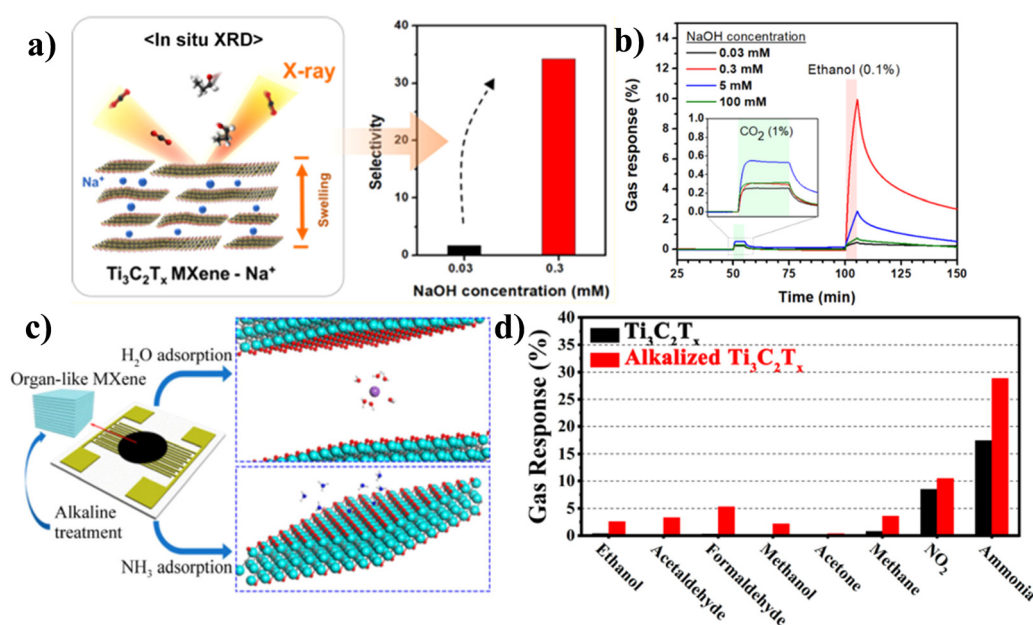
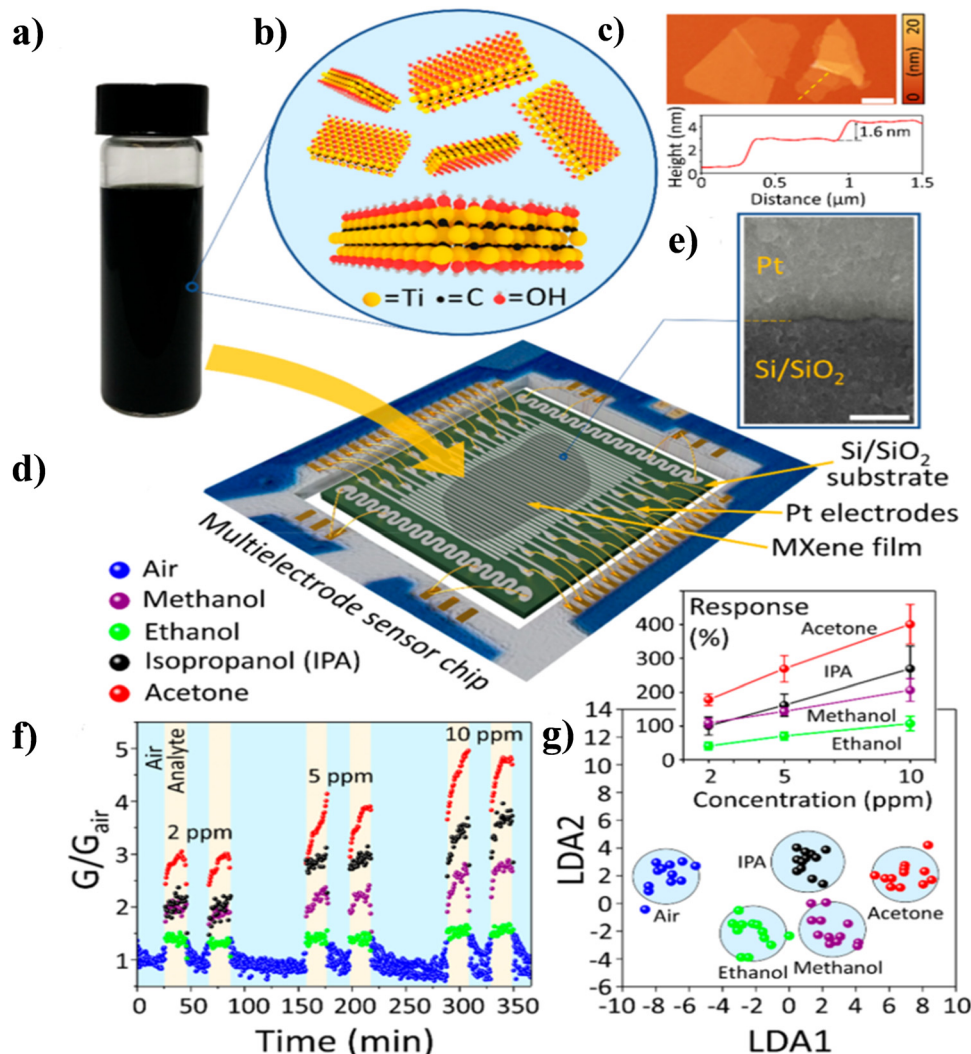


Fig. 6 (a) Gas sensor schematic based on  $\text{Ti}_3\text{C}_2\text{T}_x$ , where mM stands for  $\text{mmol L}^{-1}$ , (b) gas response of  $\text{Ti}_3\text{C}_2\text{T}_x$  sensors with different concentrations of NaOH, inset: magnified gas response of  $\text{CO}_2$ . Reproduced with permission from ref. 93 Copyright 2019. American Chemical Society, (c) schematic of an organ-like  $\text{Ti}_3\text{C}_2\text{T}_x$ -based gas sensor with alkaline treatment, (d) selectivity test of alkalized  $\text{Ti}_3\text{C}_2\text{T}_x$  and  $\text{Ti}_3\text{C}_2\text{T}_x$  with a 100 ppm concentration to various test gases. Reproduced with permission from ref. 79 Copyright 2019. American Chemical Society.







**Fig. 7** A partially oxidised  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene film's gas sensing capabilities on a multisensor chip: (a) image of a water-based, stable delaminated MXene solution, (b) monolayer  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene flakes' schematic structure, (c)  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene flakes on  $\text{Si}/\text{SiO}_2$  as depicted in an AFM image with scale bar 1  $\mu\text{m}$ , (d) schematic of a multielectrode chip with a coating of drop-cast MXene flakes, (e) SEM image of a MXene film with contact area between  $\text{Si}/\text{SiO}_2$  substrate and Pt electrode, (f) variation of MXene  $G/G_{\text{air}}$  with time, (g) the multisensor array vector signals are anticipated by LDA into a two-component taste diagram for three organic vapours (10 ppm) and dry air; the circles associated to the gases are constructed with a 0.7 confidence around the relevant gravity centres (Main figure), dependence of the chemiresistive response with different concentration of gases (inset). Reproduced with permission from ref. 95 Copyright 2020. American Chemical Society.

showed a high response and excellent selectivity for  $\text{NH}_3$ .<sup>99</sup> The heat treatment of the detecting ceramic tube, which eliminates the adsorbed water and partially oxidizes the material at a temperature of 280  $^\circ\text{C}$ , is an essential aspect of this work. The  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene-280 has a 147% response to 500 ppm  $\text{NH}_3$  in ambient conditions, whereas the equivalent response/recovery time are 67/157 s, respectively.<sup>99</sup>

The electrochemical performance of the 2D  $\text{Ti}_3\text{C}_2\text{T}_x$  sheet decorated with Pt nanoparticles (PtNPs) was studied by Lorencova *et al.*<sup>100</sup> The findings demonstrated that  $\text{Ti}_3\text{C}_2\text{T}_x/\text{PtNP}$  nanocomposite exhibited significantly superior and more stable redox activity in an anodic potential window compared to GCE treated with pure  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene. The  $\text{H}_2\text{O}_2$  sensor fabricated with  $\text{Ti}_3\text{C}_2\text{T}_x/\text{PtNP}$  on GCE provided LOD of 448 nM

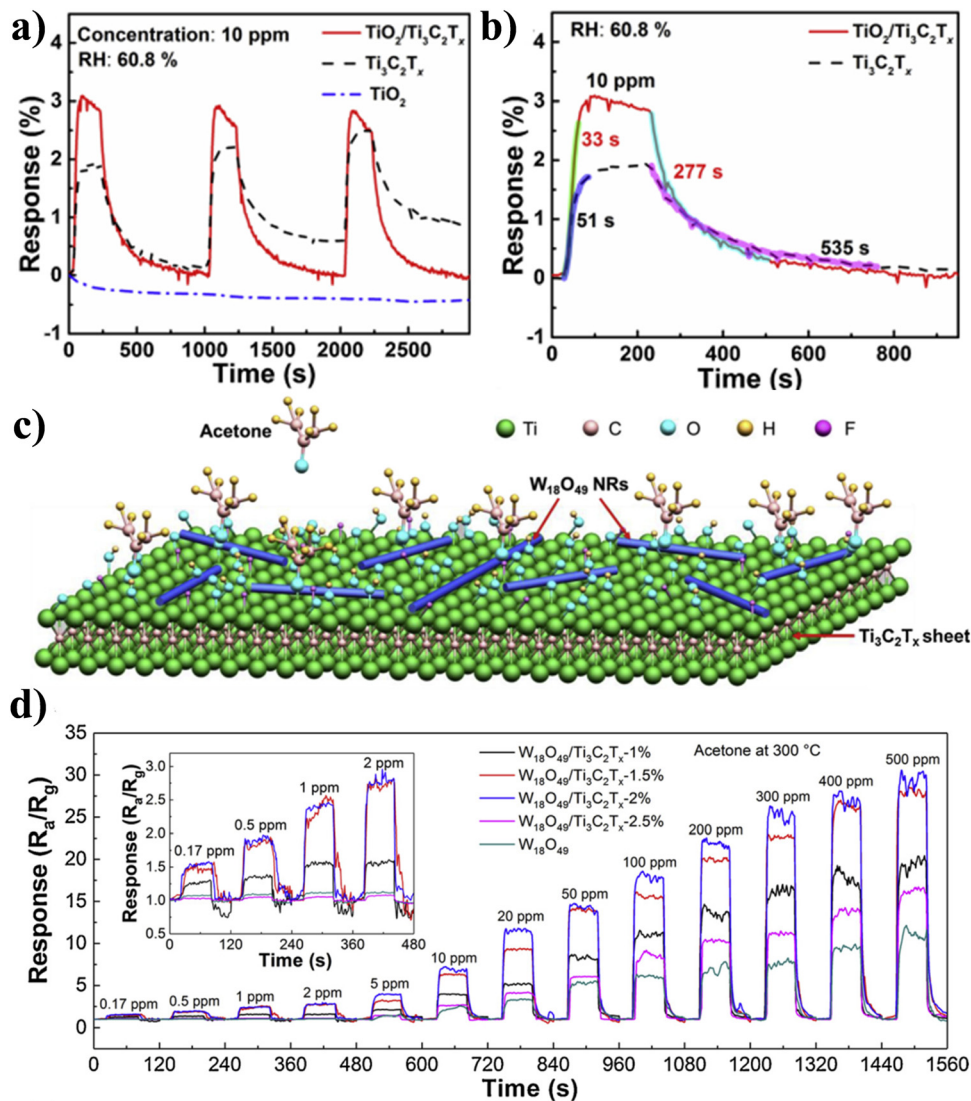
and a potential at which reduction begins of +250 mV (*vs.*  $\text{Ag}/\text{AgCl}$ ), in contrast to 883 mV and 160 mV observed for  $\text{Ti}_3\text{C}_2\text{T}_x$  modified GCE. A flexible hydrogen sensor was also fabricated by Zhu *et al.*, employing  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene that had been modified with the noble metal palladium (MXene@Pd CNC).<sup>96</sup> This sensor had a response time of  $(32 \pm 7)$  s and a sensitivity range of  $S = (23 \pm 4)\%$  to 4%  $\text{H}_2$ .

In summary, functionalized  $\text{Ti}_3\text{C}_2\text{T}_x$  MXenes hold great promise for gas sensors due to their versatility and tunable surface chemistry, offering distinct advantages and potential drawbacks. One significant advantage is their enhanced selectivity and sensitivity towards specific gases. By introducing functional groups like  $-\text{OH}$ ,  $-\text{F}$ , or  $-\text{NH}_2$ , the MXene surface can be tailored to interact selectively with target gas molecules,









**Fig. 8** (a) Response/recovery curve at a concentration of 10 ppm  $\text{NH}_3$  for  $\text{TiO}_2/\text{Ti}_3\text{C}_2\text{T}_x$ ,  $\text{Ti}_3\text{C}_2\text{T}_x$ , and  $\text{TiO}_2$  gas sensors, (b) response and recovery times of the  $\text{Ti}_3\text{C}_2\text{T}_x$  and  $\text{TiO}_2/\text{Ti}_3\text{C}_2\text{T}_x$  gas sensors. Reproduced with permission from ref. 81 Copyright 2019. Elsevier, (c) schematic of reaction between acetone and  $\text{Ti}_3\text{C}_2\text{T}_x/\text{W}_{18}\text{O}_{49}$  composite and (d) response–recovery curves of different sensors at a concentration of 0.17–500 ppm acetone at 300 °C temperature. Inset: Response–recovery curves towards 0.17–2 ppm acetone (enlarged view). Reproduced with permission from ref. 105 Copyright 2019. Elsevier.

oxidation process. This was discovered after it was established that oxidation had brought about changes in structure and composition. Calculations using the first principles of density functional theory (DFT) were carried out, and the findings revealed that the adsorption capacity of Ti atom defect sites for gas molecules was significantly improved, particularly with respect to  $\text{NO}_2$ . Meanwhile, a reducing agent known as  $\text{Ti}_3\text{C}_2\text{T}_x$  was utilized to assist in the process of GO reduction. The gas sensing performance was further improved by forming a  $\text{Ti}_3\text{C}_2\text{T}_x/\text{TiO}_2/\text{rGO}$  heterostructure, which resulted in high sensitivity, low level of detection limit, and a remarkable selectivity to  $\text{NO}_2$ , reaching up to 19.85% for 5 ppm  $\text{NO}_2$  at ambient temperature. All of these improvements were made possible by the formation of the heterostructure.

Since polymers are sensitive, cheap, versatile, and may be used at room temperature, they have frequently been used to

fabricate  $\text{Ti}_3\text{C}_2\text{T}_x$  composites. Flexible gas sensors based on the  $\text{Ti}_3\text{C}_2\text{T}_x/\text{polyaniline}$  (PANI) nanocomposite were studied by Zhao *et al.* using density functional theory in conjunction with electro-sensitive experiments on large samples.<sup>104</sup> This composite sensing material showed a high sensitivity for ethanol (41.1% at 200 ppm) and fast response/recovery time (0.4/0.5 second) at room temperature, as shown in Fig. 10(a) and (b), which makes it the next-generation sensing material that can quickly detect real-time VOC gases. This is because the properties of composites and highly active  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene work synergistically with one another. To track  $\text{NH}_3$  volatilization in farming operations, Li *et al.* report the development of a polyaniline (PANI)/ $\text{Ti}_3\text{C}_2\text{T}_x$  hybrid sensitive film-based flexible chemiresistive gas sensor.<sup>114</sup> An *in situ* method of self-assembly was utilized during the process of depositing the hybrid film

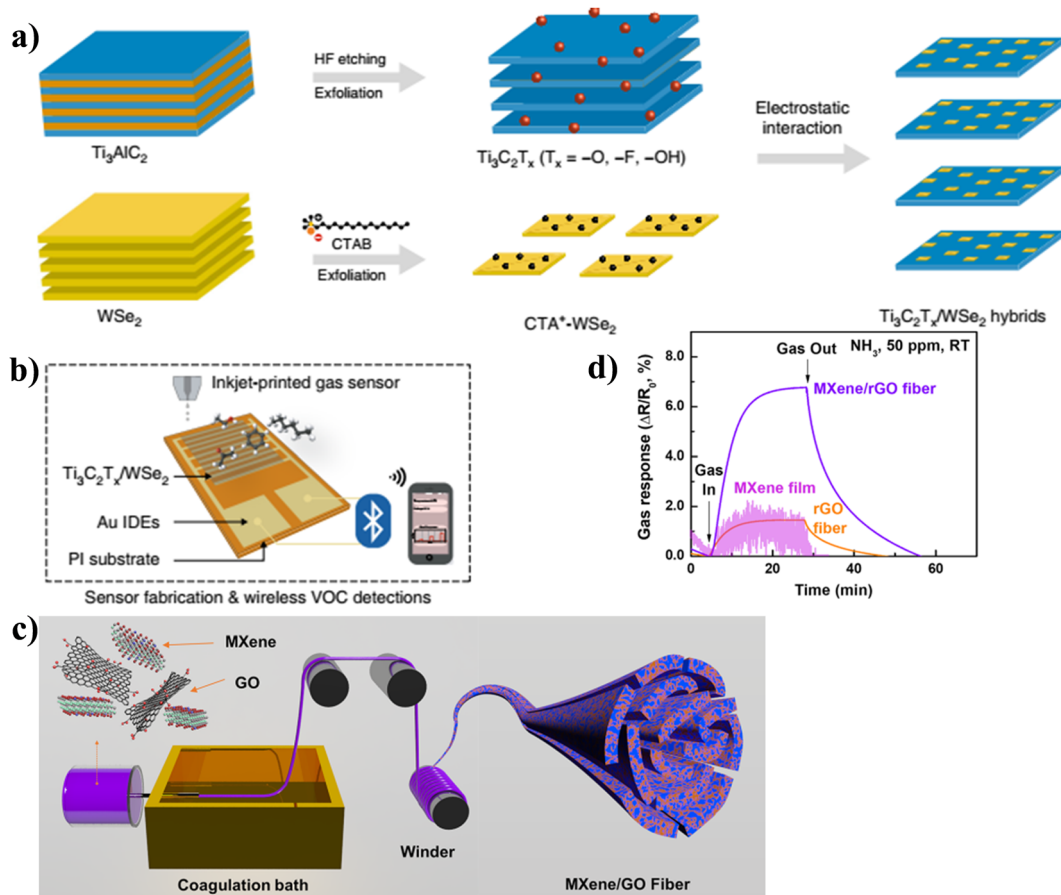


Fig. 9 (a) A schematic representation of the steps involved in the preparation of  $\text{Ti}_3\text{C}_2\text{T}_x/\text{WSe}_2$  nanohybrids, (b) illustration of inkjet-printed gas sensors for the detection of VOC using a wireless monitoring system. Reproduced with permission from ref. 102 Copyright 2020. Springer Nature (Open Access), (c) schematic of the spinning process for MXene/GO hybrid fiber, and (d) comparison of the gas response of MXene film, rGO fiber, and MXene/rGO hybrid fiber (40 wt% MXene). Reproduced with permission from ref. 112 Copyright 2020. American Chemical Society.

onto the flexible polyimide substrate, as shown in Fig. 10(c). High sensitivity, excellent repeatability, a low detection limit, and strong air stability are all characteristics of this sensor, which is enabled by the gas-sensing enhancing effects of the PANI/ $\text{Ti}_3\text{C}_2\text{T}_x$  Schottky junction and the enhanced protonation degree of PANI in the hybrids. Particularly, the sensor demonstrates outstanding  $\text{NH}_3$ -sensing properties in situations with relative humidity (RH) of 20–80% at a 10–40 °C temperature range. This makes it attractive for real-world agricultural applications because it can operate in a wide temperature range. Wang *et al.* investigated the possibility of using a conductive poly(3,4-ethylenedioxythiophene) doped with poly(styrene sulfonic acid) (PEDOT:PSS) composite  $\text{Ti}_3\text{C}_2\text{T}_x$  in a gas sensing application, as shown in Fig. 10(d).<sup>115</sup> In comparison to the pristine materials, the  $\text{Ti}_3\text{C}_2\text{T}_x/\text{PEDOT:PSS}$  sensor, which was fabricated using the process of drop-coating, exhibited superior sensing behaviors when exposed to VOC vapors at ambient temperature. They also investigated the effect of composite ratio on gas sensing performance, and the findings revealed that the ideal mass ratio for PEDOT:PSS and  $\text{Ti}_3\text{C}_2\text{T}_x$  was 4 : 1. This ratio produced the maximum response from both of these gas sensing components. Recently, Chen *et al.* reported a

nanocomposite of  $\text{Ti}_3\text{C}_2\text{T}_x/\text{MXene}$  and polypyrrole (PPy) by using *in situ* polymerization reaction for gas sensing application.<sup>116</sup> The PPy/MXene-12, a nanocomposite-based gas sensor, displayed the best possible gas-detecting performance. It had a high response of 31.9% to 100 ppm  $\text{NH}_3$ , a low detection limitation, and unflinching selectivity.

In summary, the  $\text{Ti}_3\text{C}_2\text{T}_x$  composites-based gas sensors offer a range of advantages and drawbacks, necessitating innovative solutions for their optimal performance. One significant advantage is their improved conductivity and stability compared to pristine  $\text{Ti}_3\text{C}_2\text{T}_x$ , making them highly suitable for practical gas sensing applications. These composites often integrate  $\text{Ti}_3\text{C}_2\text{T}_x$  with other materials like polymers, MOs, or carbon-based nanomaterials, harnessing the synergistic effects of each component. This enhances the sensor's electrical properties and provides a larger surface area for gas adsorption, leading to enhanced sensitivity and response times. However, a notable drawback is the potential loss of selectivity when using composites, as the additional materials may introduce cross-sensitivity to various gases. To address this, researchers are actively developing advanced composites with tailored properties that maintain or even improve selectivity while preserving





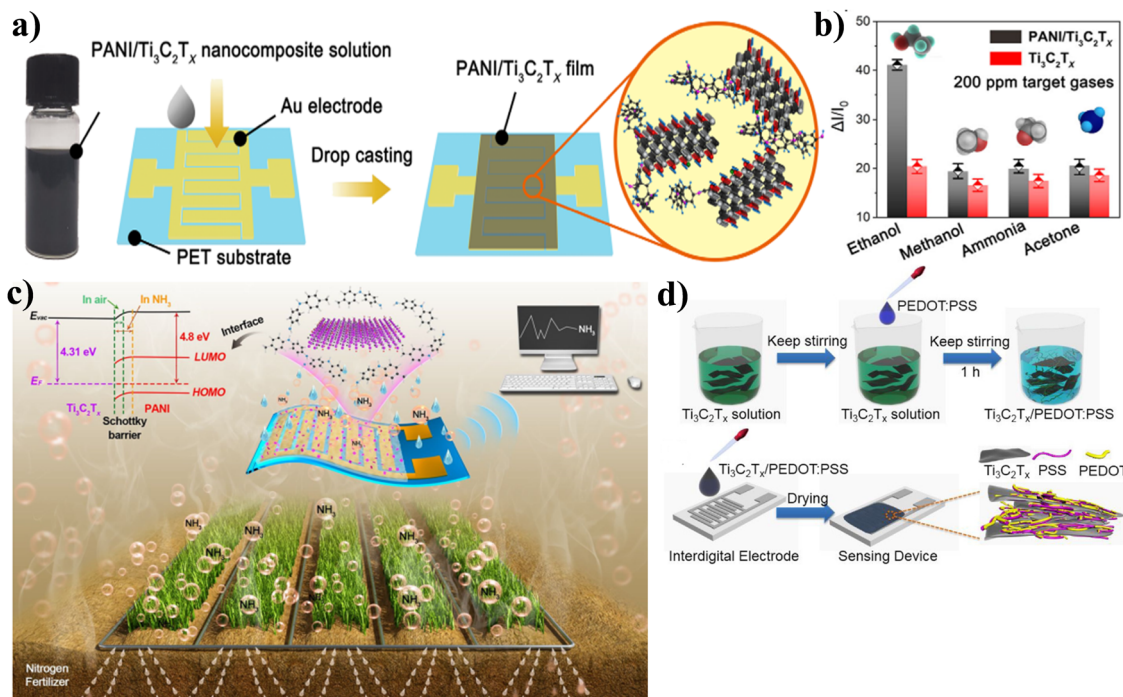


Fig. 10 (a) Interdigitated electrode schematic before and after coating with PANI/Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> nanocomposites, (b) selectivity of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> and PANI/Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>-based flexible sensors exposed to 200 ppm. Reproduced with permission from ref. 104 Copyright 2019. John Wiley & Sons (Open Access), (c) agricultural NH<sub>3</sub> volatilization monitoring based on Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/PANI NH<sub>3</sub> sensor. Reproduced with permission from ref. 114 Copyright 2020. Elsevier, (d) schematic of fabrication of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/PEDOT:PSS materials and gas sensor devices. Reproduced with permission from ref. 115 Copyright 2020. Elsevier.

high conductivity. Surface modification techniques and precise control over the composition and morphology of the composite materials allow for a fine-tuning of gas-sensing characteristics. Another challenge lies in the potential degradation of the composites over time due to environmental factors or harsh operating conditions. To overcome this, protective coatings or encapsulation techniques are being explored to shield the sensitive composites from external influences, thus improving their long-term stability and reliability. Moreover, ongoing research into the optimization of composite fabrication processes and the development of novel composite combinations are continuously pushing the boundaries of gas sensor technology, aiming to strike a balance between enhanced performance and selectivity, as well as long-term durability for a wide range of gas detection applications.

Recently, lots of research going on Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene based self-powered gas sensor. One of the most remarkable aspects of MXene-based gas sensors is their ability to operate without the need for external power sources, such as batteries. This is achieved through the concept of self-powering, where the interaction between the gas molecules and the MXene-based sensing layer generates electricity. Two primary mechanisms have been explored for self-powering MXene-based gas sensors.

(1) Piezoelectric effect: when gas molecules adsorb or react with the MXene surface, they induce mechanical deformation or strain in the sensing layer. This strain can be harvested as piezoelectric energy, which is then converted into an electrical

signal. This approach allows for the continuous and sustainable operation of gas sensors without the need for batteries.

(2) Triboelectric effect: in the triboelectric effect, friction or contact between the gas molecules and the MXene surface generates static electricity. This effect can also be harnessed to power gas sensors. As gas molecules interact with the MXene layer, they create charge imbalances that can be tapped into for sensing purposes.

Sardana *et al.* reported a self-powered humidity sensor using an electrospun anisotropic triboelectric nanogenerator (A-TENG) composed of aligned Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene nanofibers (NFs) and cellulose acetate (CA) NFs.<sup>117</sup> Significantly, anisotropic structure of TENG displays its potential in sensitive moisture detection upon fast adsorption/desorption of water molecules due to increased pore length of prepared NFs. They also demonstrated the applied application of detecting the skin moisture. The same group also reported, a new kind of MXene/TiO<sub>2</sub>/C-NFs heterojunction-based sensory component for detection of NH<sub>3</sub> by using cellulose nanofibers (C-NFs) as a substrate. At room temperature, the proposed sensor shows excellent reproducibility, high selectivity, and sensitivity toward NH<sub>3</sub> (1–100 ppm) along with a fast response/recovery time (76 s/62 s).<sup>118</sup> Wang *et al.* demonstrated self-powered and low-temperature resistant Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene-modified electronic-skin (e-skin) for multifunctional sensing.<sup>119</sup> The reported e-skin displays decent sensitivity to pressure (8(1.29 mV Pa<sup>-1</sup>) and frequency (5.60 V Hz<sup>-1</sup>) at a low temperature (–15 °C). In the meantime, utilizing this flexible e-skin, they successfully demonstrated temperature sensing over the range





from  $-15\text{ }^{\circ}\text{C}$  to  $25\text{ }^{\circ}\text{C}$  with a sensitivity of  $76.6\text{ nA cm}^{-2}\text{ }^{\circ}\text{C}^{-1}$ . Gasso *et al.* reported  $\text{SnO}_2/\text{Ti}_3\text{C}_2\text{T}_x$ -MXene nanocomposite-based self-powered gas sensor for  $\text{NO}_2$  sensing. The fabricated sensor has detection limit of  $0.03\text{ ppb NO}_2$  and power consumption as low as  $1.2\text{ }\mu\text{W}$ . Moreover, they also reported  $\text{SnO}_2/\text{MXene}$  nanocomposite-based piezoelectric pressure sensor (PPs) with a high sensitivity of  $2.088\text{ kPa}^{-1}$  under the pressure range of  $1.63\text{--}6.23\text{ kPa}$  with a fast response time ( $265\text{ ms}$ ) and recovery time ( $75.5\text{ ms}$ ).<sup>120</sup> Wang *et al.* reported high-performance  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene/tungsten oxide nanofibers-based  $\text{NO}_2$  sensor. The as fabricated self-powered  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene/ $\text{WO}_3$  sensor driven by TENG has an outstanding response at room temperature ( $\Delta U_s/U_{sa} = 510\%$  at  $50\text{ ppm}$ ) for  $\text{NO}_2$  gas, which is 15 times larger than that of the resistive MXene/ $\text{WO}_3$  sensor.<sup>121</sup>

While MXene-based self-powered gas sensors have made significant strides, ongoing research is focused on further enhancing their sensitivity, selectivity, and stability. Additionally, efforts are underway to reduce production costs and facilitate large-scale manufacturing for wider adoption. In conclusion, MXene-based self-powered gas sensors are poised to play a pivotal role in shaping the future of gas detection technology. Their unique combination of material properties, self-powering mechanisms, and diverse applications make them a promising solution for addressing environmental, industrial, and healthcare challenges. As research in this field continues to evolve, we can anticipate even more sophisticated and accessible MXene-based gas sensors that contribute to a safer and healthier world.

## 7. MXene gas sensor: theoretical approach

The intricacy of the sensing mechanism employed by MXene sensors introduces considerable difficulties when attempting to fine-tune them through experimental methods. MXene sensors are equipped with a sophisticated and multifaceted system for detecting various environmental changes or target analytes, and this complexity can make it a formidable task to optimize their performance through practical experimentation. This complexity arises from the intricate interplay of materials and physical processes within the sensor, requiring a deep understanding of its underlying principles to effectively modify and enhance its sensing capabilities. Consequently, researchers face significant challenges in achieving the desired sensor performance due to the complicated nature of the MXene sensing mechanism, which necessitates a meticulous and thorough approach to experimentation and tuning. Hence, there exists a requirement for atomic-level modeling, specifically utilizing techniques such as density functional theory (DFT) and molecular dynamics (MD), to complement the empirical data and advance our understanding of the interactions between MXene materials and gas analytes.

The first computational study was conducted by Yu *et al.*, who demonstrated the potential of MXenes as a gas sensor using monolayer  $\text{Ti}_2\text{CO}_2$ .<sup>122</sup> They investigated the interaction behavior of  $\text{H}_2$ ,  $\text{N}_2$ ,  $\text{CO}_2$ ,  $\text{CO}$ ,  $\text{NH}_3$ ,  $\text{O}_2$ ,  $\text{NO}_2$ , and  $\text{CH}_4$  gas

molecules on the semiconductor  $\text{Ti}_2\text{CO}_2$ . Because  $\text{Ti}_2\text{CO}_2$  is the only one among its counterparts [ $\text{Ti}_2\text{C}$ ,  $\text{Ti}_2\text{CF}_2$ , and  $\text{Ti}_2\text{C}(\text{OH})_2$ ] that exhibits semiconductor properties, the researchers focused their investigation on  $\text{Ti}_2\text{CO}_2$  through first-principles simulations. Out of all the gases studied,  $\text{NH}_3$  is the sole gas that chemisorbs onto the surface of the  $\text{Ti}_2\text{CO}_2$  MXene. It accomplishes this by donating a relatively substantial charge of  $0.174\text{ }e$  and establishing a N-Ti bond. In DOS analysis, there is a significant overlap of electronic charges, leading to orbital mixing and substantial charge transfer between  $\text{NH}_3$  and  $\text{Ti}_2\text{CO}_2$ . This observation strongly indicates chemisorption, where chemical bonds are formed between  $\text{NH}_3$  and  $\text{Ti}_2\text{CO}_2$ . Conversely, when examining other gas molecules, it was evident that they exhibited significantly lower gas adsorption energies and charge transfer compared to  $\text{NH}_3$ . This points to the absence of overlapping electronic charges and signifies weak interactions between these molecules and the  $\text{Ti}_2\text{CO}_2$  surface. The adsorption energy of  $\text{NH}_3$  on  $\text{Ti}_2\text{CO}_2$  was determined to be  $-0.37\text{ eV}$ , which is quite less as compared to  $\text{Ti}_2\text{C}(\text{OH})_2$  [ $-0.48\text{ eV}$ ],  $\text{V}_2\text{CO}_2$  [ $-0.81\text{ eV}$ ] and analogous to  $\text{Ti}_3\text{C}_2\text{O}_2$  [ $-0.34$ ]. The higher sensitivity of  $\text{Ti}_2\text{CO}_2$  toward  $\text{NH}_3$  was confirmed by calculating  $I$ - $V$  curves before and after absorption of gas. Xiao *et al.* investigated the interactions of various gases, including  $\text{NO}$ ,  $\text{CO}$ ,  $\text{H}_2$ ,  $\text{CO}_2$ ,  $\text{O}_2$ ,  $\text{N}_2$ , and  $\text{CH}_4$ , with  $\text{Zr}_2\text{CO}_2$  MXene.<sup>123</sup> Their findings revealed that  $\text{NH}_3$  exhibited strong chemisorption characterized by a noticeable charge transfer  $0.188\text{ }e$  and a substantial adsorption energy  $-0.81\text{ eV}$ , whereas other gases were primarily physisorbed. The authors anticipated a similar response for  $\text{M}_2\text{CO}_2$  (where  $\text{M} = \text{Sc}$ ,  $\text{Ti}$ ,  $\text{Zr}$ , and  $\text{Hf}$ ) due to their analogous atomic and electronic structures. Additionally, it was observed that the transition from chemisorption to physisorption in  $\text{NH}_3$  adsorption on  $\text{Zr}_2\text{CO}_2$  occurred when two additional electrons were introduced into the MXene sheet, offering a practical means to release the gas molecule. In a subsequent study, Wang *et al.* conducted a comprehensive analysis of  $\text{Hf}_2\text{CO}_2$ 's performance in detecting multiple gases, including  $\text{H}_2$ ,  $\text{O}_2$ ,  $\text{NO}_2$ ,  $\text{SO}_2$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{HCN}$ ,  $\text{NH}_3$ , and  $\text{H}_2\text{S}$ .<sup>124</sup> Consistent with the earlier report,  $\text{Hf}_2\text{CO}_2$  exhibited remarkable sensitivity and selectivity toward  $\text{NH}_3$ , characterized by an exceptional charge transfer of  $0.146\text{ }e$  and substantial adsorption energy of  $-0.834\text{ eV}$ . Additionally, it was observed that preadsorption of the MXene surface with  $\text{H}_2\text{O}$ ,  $\text{SO}_2$ , and  $\text{CO}_2$  molecules significantly enhanced  $\text{NH}_3$  adsorption by fostering the formation of hydrogen bonds.

In addition to their experimental investigations, Kim *et al.* conducted a detailed examination of how the functional groups of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene influence its sensing capabilities.<sup>74</sup> Employing the DFT approach, they analyzed the interactions between acetone and  $\text{NH}_3$  with  $\text{Ti}_3\text{C}_2\text{T}_x$  surfaces terminated by  $-\text{OH}$ ,  $-\text{O}$ , and  $-\text{F}$  groups. Their findings indicated that  $\text{Ti}_3\text{C}_2(\text{OH})_2$  exhibited stronger binding energy with both acetone and  $\text{NH}_3$  compared to  $\text{Ti}_3\text{C}_2\text{O}_2$  and  $\text{Ti}_3\text{C}_2\text{F}_2$  MXenes. Hajian *et al.* investigated the impact of the ratio of functional groups on  $\text{NH}_3$  detection using  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene.<sup>125</sup> They examined two different ratios of  $-\text{F}$  functional groups and observed that lower ratios of  $-\text{F}$  groups led to stronger  $\text{NH}_3$  adsorption. This effect was



attributed to the smaller charge transfer between  $\text{NH}_3$  and fluorine in comparison to  $\text{NH}_3$  and oxygen. Consequently, the synthesis method and the choice of MAX phase etchant, which dictate the functional group ratios, emerged as critical factors influencing the gas-sensing performance of MXene sensors. Zhang *et al.* examined the ability of  $\text{Ti}_3\text{C}_2\text{O}_2$  nanosheets to capture formaldehyde effectively at room temperature.<sup>126</sup> The findings revealed a moderate adsorption energy of 0.45 eV and an adsorption capacity exceeding 6 mmol  $\text{g}^{-1}$ , indicating the promising potential of  $\text{Ti}_3\text{C}_2\text{O}_2$  MXene for indoor formaldehyde removal. Ma *et al.* explored  $\text{M}_2\text{CO}_2$  (where M = Sc, Ti, Zr, and Hf) MXenes to identify the most effective platforms for detecting toxic  $\text{SO}_2$ .<sup>127</sup> Their investigation revealed that monolayer  $\text{Sc}_2\text{CO}_2$  exhibited a robust chemical bond with  $\text{SO}_2$ , characterized by an adsorption energy of  $-0.646$  eV and a charge transfer of  $0.453 e$ , establishing it as a favorable material for  $\text{SO}_2$  sensing. The  $\text{M}_2\text{CO}_2$  MXene was also explored for other gas detection such as NO and CO. Regarding NO, the most significant interactions were observed between the molecule and  $\text{Sc}_2\text{CO}_2$ , likely due to orbital hybridization occurring between the MXene and the gas molecule near the Fermi level. This was substantiated by a substantial charge transfer of  $0.303 e$  and a reasonably moderate adsorption energy of  $-0.47$  eV, affirming  $\text{Sc}_2\text{CO}_2$  as a highly suitable material for NO sensing. Conversely, in the case of CO, it was primarily physisorbed onto  $\text{Sc}_2\text{CO}_2$  MXene, with a minimal charge transfer of  $0.017 e$ . However, the sensing capabilities of  $\text{Sc}_2\text{CO}_2$  MXene for CO were enhanced through the introduction of Mn dopants into the structure, resulting in a charge transfer of  $0.199 e$  and a strong adsorption energy of  $-0.85$  eV.<sup>128</sup> Banu *et al.* utilized  $\text{M}_2\text{CO}_2$  MXene for the detection of  $\text{NH}_3$  via oxygen functionalization.<sup>129</sup> Based on the detailed

DFT study, they reported the adsorption behaviour of  $\text{NH}_3$  on  $\text{Cr}_2\text{C}/\text{Fe}_2\text{C}$  went through the alteration from chemisorption ( $E_{\text{ad}} = -1.40/-1.33$  eV) to physisorption ( $E_{\text{ad}} = -0.29/-0.22$  eV). Recently Quan *et al.* reported fully flexible  $\text{Ti}_3\text{C}_2\text{T}_x/\text{WS}_2$  based gas sensor for  $\text{NO}_2$  detection at room temperature.<sup>130</sup> To delve further into the sensing mechanism, adsorption models for  $\text{NO}_2$  on  $\text{WS}_2(001)$ ,  $\text{Ti}_3\text{C}_2\text{T}_x(001)$ , and  $\text{Ti}_3\text{C}_2\text{T}_x(001)/\text{WS}_2(001)$  were computed using the DFT method. The calculated adsorption energies for  $\text{NO}_2$  molecules on the surfaces of bare  $\text{WS}_2(001)$ ,  $\text{Ti}_3\text{C}_2\text{T}_x(001)$ , and  $\text{Ti}_3\text{C}_2\text{T}_x(001)/\text{WS}_2(001)$  were found to be  $-0.20$  eV,  $-3.37$  eV, and  $-3.73$  eV, respectively. Weng *et al.* reported highly sensitive and selective  $\text{Ti}_3\text{C}_2\text{O}_2$ -based gas sensors for  $\text{NH}_3$  sensing.<sup>131</sup> Through DFT study, they calculated adsorption energy of  $\text{NH}_3$  on  $\text{Ti}_3\text{C}_2\text{O}_2$  yields an appropriate value ( $-0.42$  eV), and the charge transfer rate of  $0.18 e$ . Based on their theoretical results, only  $\text{NH}_3$  adsorbs onto the nanosheet through chemisorption. Reji *et al.* demonstrated the  $\text{Sc}_2\text{CO}_2$  MXene nanosheets for detection of VOCs using first-principles DFT calculations.<sup>132</sup> They reported that 2-propanol ( $-0.63$  eV), ethanol ( $-0.59$  eV), and acetonitrile ( $-0.51$  eV) show higher interaction with the  $\text{Sc}_2\text{CO}_2$  MXene nanosheets. At the end, they also predict that  $\text{Sc}_2\text{CO}_2$  MXene nanosheets can be utilized as a dual-mode sensor to detect potential VOC biomarkers in the exhaled breath.

## 8. Advantage and drawback of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene gas sensors and other common materials

$\text{Ti}_3\text{C}_2\text{T}_x$  MXene is a promising material for gas sensors, but like any material, it has its advantages and drawbacks when

Table 1 Advantage and drawback of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene with some common material

S. no.	Materials	Advantages	Drawbacks
1.	$\text{Ti}_3\text{C}_2\text{T}_x$ MXene based gas sensor	<ul style="list-style-type: none"> <li>✓ High sensitivity</li> <li>✓ Tunable properties</li> <li>✓ Good conductivity</li> <li>✓ Chemical stability</li> </ul>	<ul style="list-style-type: none"> <li>• Complex synthesis</li> <li>• Limited gas selectivity</li> <li>• Poor humidity sensitivity</li> </ul>
2.	Metal oxide-based gas sensors (e.g., $\text{SnO}_2$ and $\text{ZnO}$ )	<ul style="list-style-type: none"> <li>✓ Low cost</li> <li>✓ Commercial availability</li> <li>✓ Good selectivity</li> </ul>	<ul style="list-style-type: none"> <li>• High operating temperature</li> <li>• Slow response/recovery</li> <li>• Limited sensitivity</li> </ul>
3.	Organic polymer-based gas sensors	<ul style="list-style-type: none"> <li>✓ Low cost</li> <li>✓ Low power consumptions</li> <li>✓ Tailorability</li> </ul>	<ul style="list-style-type: none"> <li>• Limited sensitivity</li> <li>• Limited durability</li> <li>• Limited operating range</li> </ul>
Other 2D materials (e.g., graphene, TMDs like $\text{MoS}_2$ )			
4.	Graphene	<ul style="list-style-type: none"> <li>✓ Excellent electrical conductivity</li> <li>✓ Low noise levels</li> <li>✓ High surface area</li> </ul>	<ul style="list-style-type: none"> <li>• Limited gas selectivity.</li> <li>• Difficulty in functionalizing for specific gas detection</li> <li>• Susceptibility to environmental factors, such as humidity</li> </ul>
5.	TMDs	<ul style="list-style-type: none"> <li>✓ Good gas selectivity due to varying band structures</li> <li>✓ Layer-dependent properties for tenability</li> <li>✓ Compatibility with existing semiconductor technologies.</li> </ul>	<ul style="list-style-type: none"> <li>• Moderate surface area compared to MXenes.</li> <li>• Synthesis challenges</li> <li>• Sensitivity to environmental conditions, including humidity.</li> </ul>



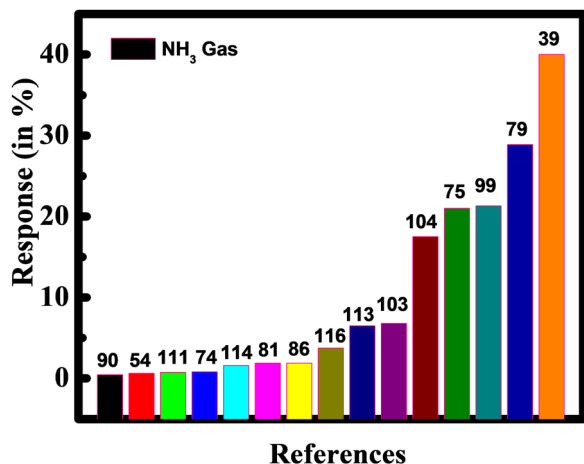


Fig. 11 Gas response of NH<sub>3</sub> gas with Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene-based gas sensors.

compared to common materials used in gas sensing applications. The comparison of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene with some common materials is given in Table 1.

In summary, Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene-based gas sensors offer unique advantages such as high surface area, tunability, and fast response times. However, they also face challenges related to synthesis complexity, moisture sensitivity, and limited gas range. The choice of gas sensor material depends on the specific application and requirements for sensitivity, selectivity, and operational conditions.

Our detailed study suggested that Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene-based gas sensors have a high response value for NH<sub>3</sub> gas. The response of NH<sub>3</sub> gas based on Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene with different literature has been shown in Fig. 11.

We have summarised the different types of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene (pure, functionalized and composite) based gas sensors in terms of sensitivity, limit of detection and working range in Table 2.

## 9. Conclusions and future prospective

MXenes are a newly discovered family of 2D materials that have been the subject of intensive research due to the exceptional properties that make them exceedingly valuable for use in various applications. MXene-based sensors have been among the most extensively researched applications because they are able to exploit the full potential of the one-of-a-kind 2D structure of MXenes. This is because MXenes have an inherently large specific surface area and surface-mediated properties that can be controlled. Thus, investigations on MXene-based gas sensors have been enhancing the selectivity and sensitivity using approaches such as composite formation, surface functionalization, and macro-structuring. The fact that the alternation of the MXene surface does not forfeit its fundamental outstanding electrical conductivity and improves its other physical and chemical properties makes it one of the most promising materials for sensors. For instance, it is conceivable to boost the adsorption energy of analytes on the

Table 2 Summary of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene-based gas sensor

MXene	MXene type	Target gas	Sensitivity in %	Limit of detection (LOD)	Working range	Ref.
Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>	Pure	Ammonia	0.21	NR	25 to 200 ppm	75
	Pure	Acetone	0.97	0.011 ppb	50 ppb to 100 ppm	74
	Pure	Nitrogen dioxide	4.5	NR	5 ppm	91
	Pure	Ammonia	0.62	NR	5 ppm	54
	Pure	Ammonia	6.13	NR	10 to 700 ppm	86
	Pure	Ammonia	1.22	NR	1 to 100 ppm	133
	Pure	Methane	68	NR	200 to 10 000 ppm	134
	Pure	Toluene	19.32	NR	1 to 50 ppm	94
	Functionalized	Ethanol	9.99	NR	0.3 mM L <sup>-1</sup> NaOH	93
	Functionalized	Hydrogen	23 ± 4	NR	0.5 to 40% H <sub>2</sub>	96
	Functionalized	Toluene	79.5	NR	1 to 50 ppm	94
	Functionalized	Ammonia	28.87	NR	10 to 500 ppm	79
	Composite	Ethanol	14	NR	5 to 120 ppm	135
	Composite	Toluene	79.5	NR	1 to 50 ppm	94
	Composite	Hydrogen	70	NR	100 to 500 ppm	136
	Composite	Ammonia	6.2	NR	1 to 80 ppm	137
	Composite	Ammonia	3.1	NR	10 ppm	81
	Composite	Ammonia	0.4	NR	1 to 100 ppm	138
	Composite	Ammonia	24.8	NR	1 to 100 ppm	139
	Composite	Ammonia	22.3	NR	1 to 5 ppm	80
	Composite	Ammonia	40	4.29 ppb	0.5 to 100 ppm	39
	Composite	Ammonia	100.7	NR	20 ppm	140
	Composite	Toluene	11.4	NR	10 to 50 ppm	141
	Composite	Nitrogen dioxide	41.93	NR	5 to 100 ppm	142
	Composite	Nitrogen dioxide	37	125 ppb	0.125 to 5 ppm	101
	Composite	Nitrogen dioxide	165	50 ppb	0.05 to 20 ppm	143
	Composite	Acetone	0.25	0.05 ppm	0.05 to 30 ppm	144
	Composite	Acetone	52	NR	10 to 500 ppm	145
	Composite	Ethanol	27.4	NR	50 to 200 ppm	104
	Composite	Carbon dioxide	1	NR	8 to 3000 ppm	146
	Composite	Hexanal	3.4	217 ppb	10 to 40 ppm	147
	Composite	Methanol	29.6	NR	5 to 100 ppm	106



MXene surface while maintaining the material's conductivity. The aforementioned methods have proven to be successful in the majority of the research aimed at enhancing the performance of sensors.

The development of MXene-based sensors is still in its early stages; therefore, there are still issues that need to be resolved before they can be used commercially. There needs to be more information about these requirements because the performance standards and other requirements for putting these sensors on the market have not yet been developed in a systematic way. In this review, we have discussed the recent developments in the field of gas sensors based on 2D  $Ti_3C_2T_x$  from three different perspectives: etching and delamination of  $Ti_3C_2T_x$ ; pure, functional, and composite  $Ti_3C_2T_x$  applied in gas sensors; and their sensing mechanism. The  $Ti_3C_2T_x$  MXene has garnered a lot of attention and has been demonstrated to offer a lot of potential in the field of gas sensor. This is because of their one-of-a-kind structure and features. However, the application of  $Ti_3C_2T_x$  in the real world is constrained by a number of different reasons. The first difficulty is associated with the process of preparing the MXene precursor, also known as the MAX phase. In most cases, the formation of a MAX phase occurs as a result of the high-temperature processing of combustible materials in powder forms, such as titanium, aluminum, and others. To obtain a MAX powder of the desired fineness, multiple milling processes are necessary. If HF is to be used as an etchant, the handling of HF and treatment of waste must be done correctly. The second obstacle is the mass production of MXene-based sensors, which is difficult because MXene does not have sufficient mechanical stability to be processed by industrial machines. In order to overcome this obstacle, researchers have been concentrating on the fabrication of nanocomposites by combining MXenes with a variety of other materials, particularly polymers. The third obstacle is determining the ideal proportion of MXene to incorporate into a polymer matrix in order to produce a high-performance sensor. The fourth obstacle pertains to applications that take place in the real world and require sensors to be durable and functional even after being damaged. This can be accomplished by modifying the surface of the components that make up a sensor, which in most cases results in improved mechanical properties of those components. The fifth obstacle is the requirement for clean and flawless MXene surfaces, which increases the sensitivity of MXene-based sensors. It is necessary to develop etchants that are superior to both HF and HCl/LiF. In general, the focus of research efforts on this subject at the moment is on exploring the maximal capability and potential of  $Ti_3C_2T_x$  MXenes in terms of transferring their advantageous properties to sensors in order to obtain high performance of sensitivity and LOD. These aspects are absolutely necessary for the successful commercialization of MXene-based sensors. However, in order for MXenes to be successfully employed in the industry, several practical characteristics, including productivity, stability, and multifunctionality, should be examined and improved.

As a result, the area of future research should be broadened, and the primary objective should be to enhance sensor performance in terms of the variables described above so that it is

compatible with industry requirements. In order to speed up the development of next-generation sensor technologies based on MXenes, it will be necessary to address the requirements listed above for commercialization. This will eventually pave the way for the creation of low-cost, high-performance, and multimodal sensors that can be used in soft-electronics applications. We hope this work will provide a roadmap for the commercialization of  $Ti_3C_2T_x$  MXene-based gas sensors and encourage a wide range of in-depth and applicable studies in this area.

## Conflicts of interest

All authors declare that they have no conflicts of interest. We certify that the submission is original work and is not under review at any other publication.

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