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# Synergistic Impacts on Properties, Stability, and Applications of MXenes via Polymer Integration

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## Abstract

MXenes are known for their exceptionally high electrical conductivity, mechanical resilience, and versatile surface chemistry. However, these tend to oxidize under ambient conditions, posing a major hurdle in their performance in various applications. Contrary to these, polymers are mostly stable under ambient conditions, making these ideal materials to combine with MXenes to create MXene-polymer nanocomposites with enhanced higher stability against oxidation and improving MXenes functionality. This synergy can also enhance the mechanical strength, thermal stability, surface properties, and other characteristics of MXenes improving the overall performance of MXenes. This review focuses on the role of polymers in improving the properties of MXenes and mitigating their oxidation under various conditions. Polymers serve as protective barriers and improve interfacial interactions, maintaining various properties of MXenes for longer periods. The review also highlights MXene-polymer nanocomposite fabrication techniques, like solution blending, layer-by-layer assembly, in-situ polymerization, electrospinning, etc., for their effective integration. The review also explores MXene-polymer nanocomposite applications in different areas, including energy storage devices, electronics, sensors, filtration membranes, biomedical applications, etc. Finally, the review also outlines various challenges and opportunities in synthesizing MXene-polymer nanocomposites for diverse applications, emphasizing the potential of MXene-polymer synergy to open new opportunities in future hybrid materials.

**Keywords:** MXene; Polymer nanocomposites; Oxidation stability; Synthesis strategies; Synergistic effects; Applications.



## 1 1. Introduction

2 Nanocomposites have been identified as a promising way to meet the growing global demands  
3 in various sectors including energy. The combination of nanoparticles, nanofillers, and a polymer  
4 matrix material leads to improved properties like strength, conductivity, catalytic activity, etc. in  
5 these materials<sup>1</sup>. The potential of nanocomposites lies in their ability to revolutionize energy  
6 storage, conversion, and transportation technologies, which can offer more efficient and  
7 sustainable solutions for the future<sup>2</sup>. Polymers are the most popular for nanocomposite synthesis  
8 due to their versatility, easy processing, and ability to incorporate various nanofillers<sup>3</sup>. Different  
9 materials can be used as filler for the synthesis of polymers-based nanocomposites<sup>4</sup>. In this  
10 perspective, 2D MXenes are now recognized as a promising candidate<sup>5</sup>. MXenes originate from  
11 *MAX* phases, which are compounds of transition metals, by undergoing an etching process using  
12 HF or LiF/HCl acids<sup>6</sup>. Following the etching process, the *A* component is removed from the *MAX*  
13 phases, and the resulting MXenes are thoroughly washed with DI water. MXenes possess surface  
14 terminal groups such as -OH, -O, -Cl, or -F, and are commonly denoted as  $M_{n+1}X_nT_x$ , where *M*  
15 denotes a transition metal element, *X* typically denotes carbon/nitrogen/carbonitrides, and *T<sub>x</sub>*  
16 represents surface functionalities as terminal groups<sup>7</sup>.

17 MXenes have remarkable features such as high electrical conductivity<sup>8, 9</sup>, hydrophilicity<sup>10</sup>,  
18 electrochemical characteristics<sup>11, 12</sup>, adjustable band gap<sup>13, 14</sup>, and substantial surface area<sup>15</sup>. These  
19 characteristics make MXenes versatile materials having applications in fields such as energy  
20 storage<sup>8, 11, 15, 16-18</sup>, fuel cells<sup>19, 20</sup>, photodetectors<sup>14, 21</sup>, sensors<sup>22</sup>, conductive ink<sup>23</sup>, 3D printing<sup>24, 25</sup>,  
21 smart windows<sup>27</sup>, electromagnetic interference (EMI)<sup>28, 29</sup>, etc. Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene stands out as  
22 the most widely recognized member of the MXene family. High electrical conductivity, tailored  
23 surface, thermal stability, mechanical strength, etc. make it the favorite member of the MXene  
24 family. In addition to Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>, the MXene family includes other potential members, such as  
25 Ti<sub>2</sub>CT<sub>x</sub><sup>30</sup>, V<sub>2</sub>CT<sub>x</sub><sup>18, 31, 32</sup>, Nb<sub>2</sub>CT<sub>x</sub><sup>33</sup>, etc. These MXenes, each having unique characteristics, offer a  
26 wide range of properties useful in diverse potential applications<sup>34</sup>. MXenes, including Ti<sub>2</sub>C, V<sub>2</sub>C,  
27 Nb<sub>2</sub>C, Mo<sub>2</sub>TiC<sub>2</sub>, and Mo<sub>2</sub>Ti<sub>2</sub>C<sub>3</sub>, showcase distinctive characteristics distinguishing them from the  
28 widely studied Ti<sub>3</sub>C<sub>2</sub>. For example, Ti<sub>2</sub>C has thinner layers, offering a slightly larger bandgap and  
29 rapid ion transport, making it suitable for photothermal therapy<sup>35</sup>, energy storage applications<sup>36</sup>,  
30 electrocatalysts for water splitting<sup>37</sup>, etc. V<sub>2</sub>C demonstrates Superior redox properties due to the



variable oxidation states of vanadium, improving its performance in pseudo capacitors and catalytic reactions<sup>38</sup>. Similarly, Nb<sub>2</sub>C is known for its superior electrochemical durability in aqueous and organic electrolytes, making it highly suitable for robust energy storage<sup>39, 40</sup>, and photocatalytic applications<sup>41</sup>. Additionally, Nb<sub>2</sub>C MXene demonstrates good electrical conductivity and improved wettability, attributed to its lower Fermi energy level relative to Ti<sub>3</sub>C<sub>2</sub><sup>39</sup>. In the case of dual-transition metal MXenes (M<sub>2</sub>'M''C<sub>2</sub>), structurally stable Mo<sub>2</sub>TiC<sub>2</sub> combines the enhanced catalytic performance of Mo with the structural integrity of Ti, offering improved HER/OER performance<sup>42</sup> and N<sub>2</sub> reduction reaction activity<sup>43</sup>. Similarly, Mo<sub>2</sub>Ti<sub>2</sub>C<sub>3</sub>, with its thicker multilayer structure, offers tunable conductivity and thermal stability, positioning it as a promising material for thermal management and electronics. Mo<sub>2</sub>Ti<sub>2</sub>C<sub>3</sub> MXene manifests elevated photothermal conversion efficiency due to its substantial optical absorption across a wide spectral range, and layered structure, which facilitates efficient heat transfer and energy dissipation<sup>44</sup>. Partially oxidized Mo<sub>2</sub>Ti<sub>2</sub>C<sub>3</sub> MXene has demonstrated significant potential for energy storage applications due to its enhanced electrochemical properties and structural stability<sup>45</sup>.

MXenes boast various remarkable properties, however, these are vulnerable to oxidative degradation when exposed to ambient conditions or during processing, which restricts their practical application<sup>46</sup>. Therefore, enhancing oxidation stability is crucial for their broader adoption in real-world uses. Various methods have been proposed to enhance the oxidation stability of MXenes. These methods include storing MXenes at low temperatures in Ar atmosphere<sup>47</sup>, or in eutectic solvents<sup>48</sup>, using sodium L-ascorbate<sup>49</sup>, or integrating MXenes into polymer blends<sup>50, 51</sup>. The use of polyanions for preservation has shown promising results in minimizing the MXenes oxidation, as this process usually begins at the edges of the material<sup>52</sup>. MXenes treated with antioxidants have demonstrated better stability under ambient conditions, allowing their use in energy storage applications for more than 80 days<sup>53</sup>. Among these approaches, MXene-polymer hybrids or nanocomposites stand out most favorably as they provide various functionalities to these hybrid materials. However, the techniques of passivation or blending may lead to decreased electrical conductivity compared to pure MXenes.

Polymers are recognized for their outstanding capability to be processed and shaped. Incorporating MXenes into polymers can enhance and customize their characteristics for particular uses. MXene-



1 polymer nanocomposites can improve mechanical attributes, including flexibility, tensile strength,  
2 and toughness<sup>54, 55</sup>. MXenes are prone to oxidation and deterioration in typical environmental  
3 conditions<sup>56</sup> but polymers can form a protective barrier around the MXene flakes, which increases  
4 their stability against oxidation<sup>50, 51</sup>. Additionally, the polymers mixed with MXenes provide  
5 numerous possibilities for functionalization and alteration<sup>57</sup>. MXene-polymer nanocomposites  
6 have found applications in flexible electronics<sup>24, 58-60</sup>, self-healing sensors<sup>61</sup>, 3D printing<sup>62-64</sup>,  
7 energy storage<sup>50, 65</sup>, anti-corrosion<sup>66, 67</sup>, fire retardants<sup>68</sup>, water purification/treatment<sup>69-71</sup>, solar  
8 cells<sup>72, 73</sup>, and antibacterial applications<sup>74-76</sup>.

9 MXene-polymer nanocomposites can be prepared using methods, such as solution casting<sup>68, 77</sup>,  
10 solution blending<sup>78</sup>, electrospinning<sup>79, 80</sup>, in-situ polymerization<sup>81, 82</sup>, thin film coatings or polymer  
11 lamination<sup>50</sup> or fibers<sup>83, 84</sup>, etc. Some of the popular polymers which are hybridized with MXene  
12 include polyvinyl alcohol (PVA)<sup>85</sup>, Polydimethylsiloxane (PDMS)<sup>86</sup>, poly(3,4-  
13 ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS)<sup>87, 88</sup>, polyaniline (PANI)<sup>89</sup>,  
14 polypyrrole (PPy)<sup>90</sup>, etc. The polymers can serve as intercalants or spacers within MXene-polymer  
15 nanocomposites<sup>16, 91</sup>.

16 Some earlier reviews on MXene-polymer composites are available; however, these primarily focus  
17 on synthesis and general applications<sup>92, 93</sup>, or the role of MXenes as fillers<sup>94</sup>, and a few are  
18 outdated<sup>95</sup>. This article uniquely highlights the synergistic effects of MXene-polymer integration,  
19 showcasing enhancements in mechanical strength, conductivity, and thermal stability. By  
20 emphasizing these synergistic effects and the latest advancements, this review provides a  
21 comprehensive and up-to-date perspective on their advanced applications, filling the gaps left by  
22 previous studies.

## 2. MXenes synthesis

24 The synthesis of 2D MXenes was first achieved in 2011 by etching  $Ti_3AlC_2$  using a highly  
25 concentrated acid. This top-down approach involves removing the "A" layer from the MAX  
26 phases. A strong acid like HF effectively breaks the M-A metallic bond leading to the formation  
27 of layered MXene structures. The reaction mechanism of selective etching using HF is as  
28 follows<sup>96</sup>:



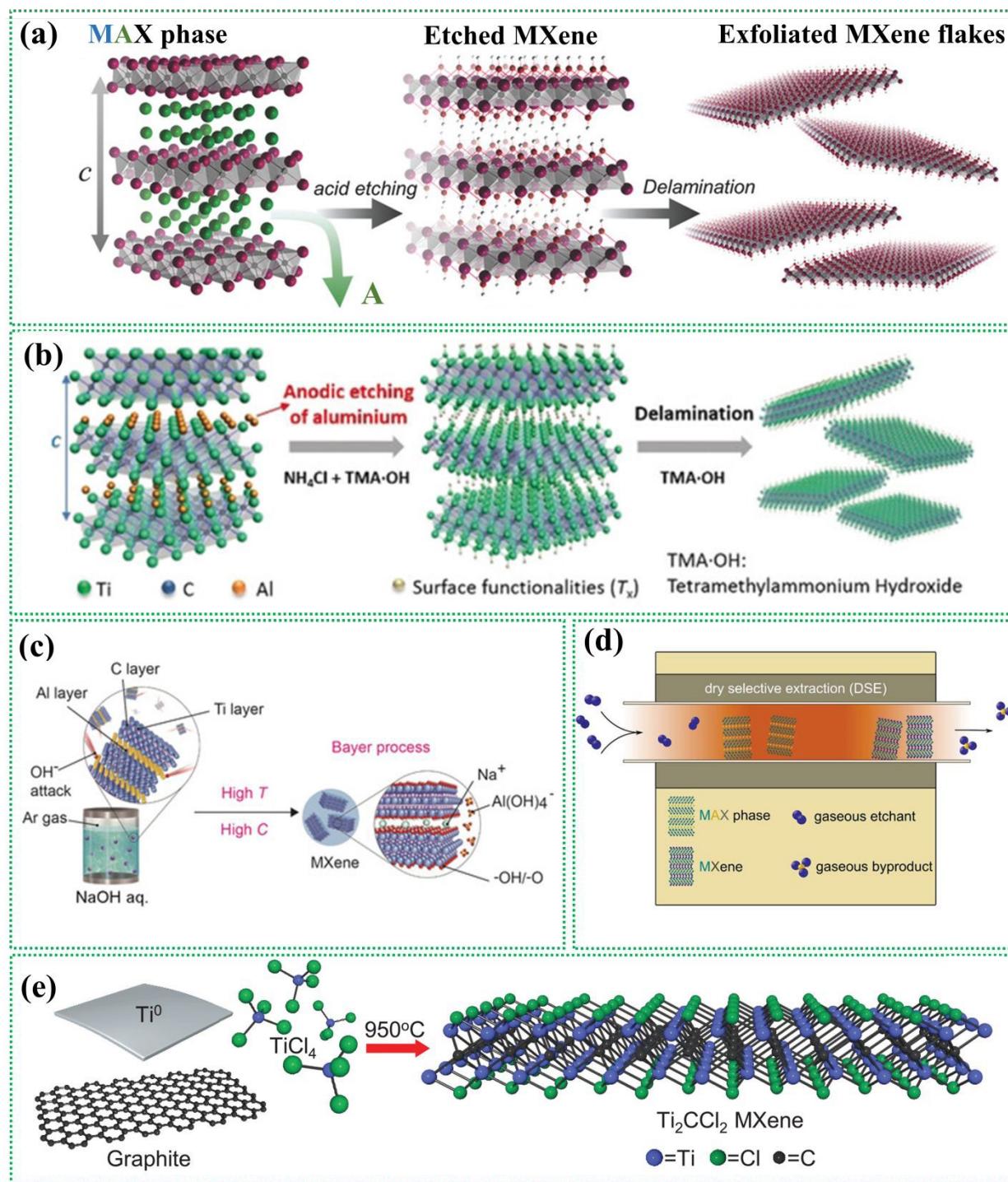


2 During the HF etching process, Al (A layer) removal causes surface terminations, leading to the  
3 functionalization of the M layer. The chemical etching in an acidic medium inevitably results in  
4 defect sites in synthesized MXene flakes. These defect sites play a key role in the oxidation of  
5 MXenes and reduce their self-life to a few days in an ambient environment, limiting their extensive  
6 use. Later many synthesis routes were developed but selective etching methods using fluoride-  
7 containing agents in an acidic medium were widely used<sup>97</sup>. The reaction time, temperature, and  
8 acid concentration affect the quality and quantity of resultant MXenes.

9 Despite the successful synthesis of MXenes using concentrated HF etching, environmental  
10 concerns and the need for a safer, simpler method have prompted the use of mild etching agents  
11 like HCl with various fluoride salts for large-scale production. The HCl and fluoride salts mixture  
12 forms in-situ HF for etching the “A” layer in the MAX phases (Figure 1a). The MXenes  
13 synthesized using HCl have high yields, fewer defects, and resulted in higher electrical  
14 conductivity. However, the MAX phase's purity is also a crucial factor in deciding the resultant  
15 properties of MXenes<sup>98</sup>. Natu et.al reported a water-free synthesis method using polar solvents  
16 along with ammonium dihydrogen fluoride<sup>99</sup>. The etching process in this method is reported to be  
17 very slow but surprisingly the resultant MXene has only the -F group as the termination species.

18 One of the major issues associated with MXene synthesis is the use of hazardous chemicals, such  
19 as HF or in situ-produced HF from fluoride salts and strong acids, which pose significant  
20 ecological and health hazards. These chemicals can lead to hazardous waste, requiring meticulous  
21 management and disposal processes. To address these issues, researchers have been exploring  
22 environmentally friendly or less harmful methods for MXene synthesis. Recently, fluoride-free  
23 synthesis methods including the electrochemical method<sup>100</sup>, molten salts assisted etching<sup>101</sup>, the  
24 alkali etching method<sup>102</sup>, chemical vapor deposition (CVD) synthesis approach<sup>103</sup>, etc., have been  
25 developed to minimize hazardous byproducts. These methods not only mitigate safety and  
26 environmental concerns but also allow the alteration of the MXene structure and surface chemistry,  
27 making them promising approaches for scalable and eco-friendly MXene production.





**Figure 1.** MXene synthesis strategies. (a) MXene etching by fluorine-based etchants. Reproduced with permission from ref.<sup>104</sup>. Copyrights 2016, Wiley. (b) Electrochemical etching method. Reproduced with permission from<sup>100</sup>. Copyrights 2018, Wiley. (c) Alkali-assisted etching method. Reproduced with permission from ref.<sup>102</sup>. Copyrights 2018, Wiley. (d) Dry selection extraction approach. Reproduced with permission from<sup>105</sup>. (e) CVD method-based MXene synthesis using Ti, graphite, and TiCl<sub>4</sub>. Reproduced with permission from ref.<sup>103</sup>. Copyrights 2023, The American Association for the Advancement of Science.



1 The electrochemical etching method selectively removes the “A” layer from the MAX phase using  
2 non-acidic electrolytes, making it safer and more environmentally friendly than traditional acid-  
3 based methods. In a two-electrode system (Figure 1b), the bulk MAX phase (like  $Ti_3AlC_2$ ) serves  
4 as both the anode and counter electrode, with an electrolyte including ammonium chloride and  
5 tetramethylammonium hydroxide (TMAOH, pH > 9). The anode undergoes etching at room  
6 temperature, under a constant potential while the electrolyte is stirred. After a few hours, the  
7 electrolyte becomes grey-white with a gelatinous precipitate, and black powders (stacked  $Ti_3C_2T_x$ )  
8 settle at the bottom.

9 The alkali etching method employs alkali solutions (like NaOH or KOH) to selectively remove the  
10 “A” layer from the MAX phase, resulting in the synthesis of layered MXenes (Figure 1c). In this  
11 method, an alkaline solution is dissolved in argon-purged deionized water before adding the MAX  
12 phase powder. The mixture is transferred to an autoclave, sealed, and subjected to heating under  
13 an argon atmosphere for 12 hours. After the hydrothermal process, the resulting suspension is  
14 filtered, thoroughly rinsed, and dried under vacuum, producing MXene with minimal impurities  
15 and a high degree of purity. This method is considered safer and more straightforward than  
16 fluorine-based acidic etching but may yield lower amounts of MXene or require extended reaction  
17 times depending on the alkali concentration and reaction conditions.

18 These methods lead to MXene formation but exhibit low yield and are more time-consuming than  
19 fluoride-based synthesis approaches. Recently, a new approach called dry selective extraction has  
20 been proposed theoretically<sup>105</sup>. In this method, a glass ampoule filled with a known quantity of  
21 MAX phase is placed in a tube furnace at an elevated temperature (Figure 1d). Iodine vapors are  
22 then passed through the ampoule containing the MAX phase at 350°C, acting as an etchant to  
23 remove the A layer and leaving behind MXenes. It was reported that the reaction does not occur  
24 below 350°C and temperatures above 400°C result in over-etching.

25 The bottom-up synthesis methods allow precise control over material chemistry thus enabling  
26 tailored customization of material design. The bottom-up approaches include CVD method<sup>103</sup>  
27 (Figure 1e) and direct solid-state synthesis. In a recent article, Wang et al. reported Ti-based and  
28 Zr-based MXenes by combining Ti metal and graphite powder with the desired quantity of  
29  $TiCl_4$ <sup>103</sup>. The sealed ampoules containing this mixture were placed in a furnace at 950°C for 2 h to  
30 obtain MXenes. The process involved methane or  $N_2$  gas reacting with  $TiCl_4$  on the titanium



1 surface, resulting in Cl-terminated  $\text{Ti}_2\text{CCl}_2$  or  $\text{Ti}_2\text{NCl}_2$  MXenes. The proposed method is shown to  
2 have the potential for bulk production.

3 Besides these, the salt-template MXene synthesis was reported by Xiao et al. to synthesize  
4 molybdenum nitride<sup>106</sup>. In this method, a 2D template of  $\text{MoO}_3$  is prepared and coated with NaCl  
5 by annealing in an Ar atmosphere. The NaCl-coated 2D  $\text{MoO}_3$  mixture was heated to 650 °C in  
6  $\text{NH}_3$  atmosphere to yield MoN MXene. Ding et al. introduced a chemical scissor-mediated method  
7 for precise structural editing of layered transition metal carbides to synthesize MXene<sup>107</sup>. This  
8 method uses chemical scissors to open non-van der Waals gaps in MAX phases, followed by  
9 atomic replacement via diffusion of metal ion intercalants into interlayer vacancies. The scissors  
10 are also used for termination removal.

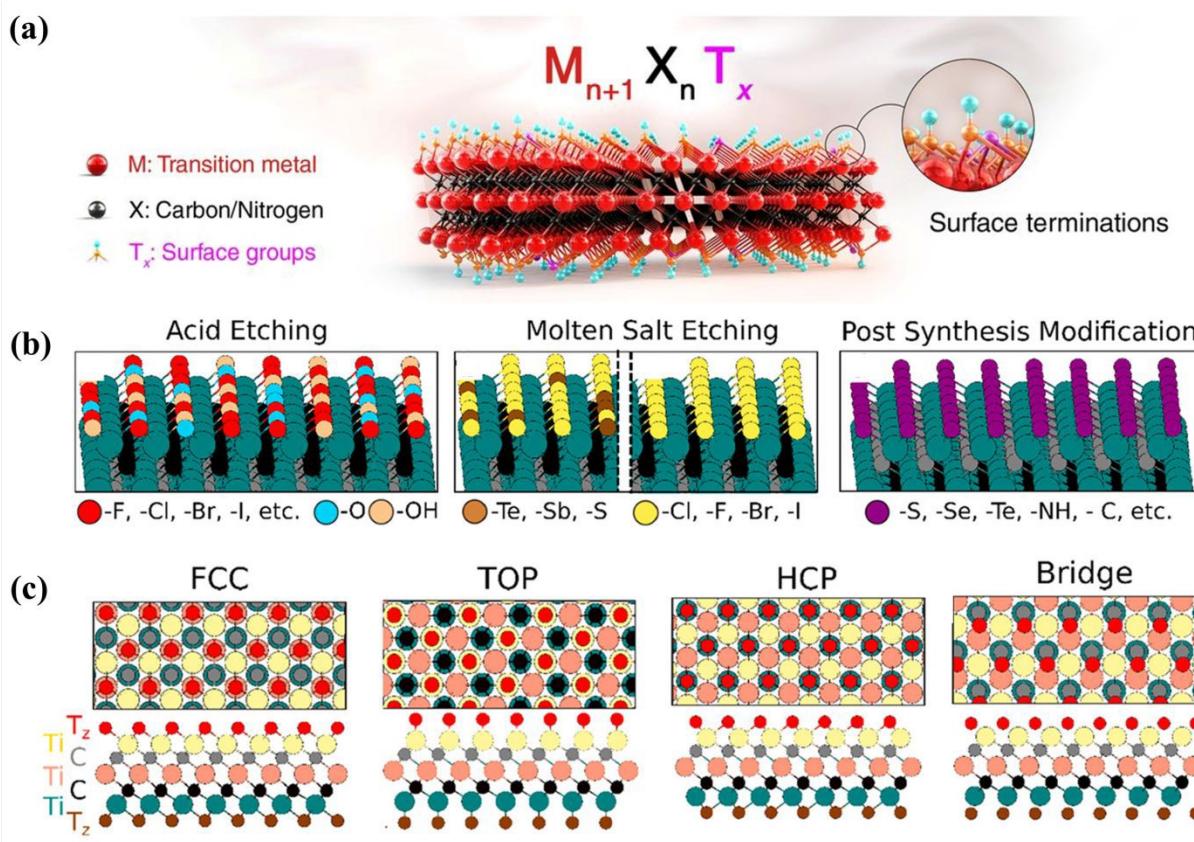
### 11     **3. MXenes structure and surface chemistry**

12 MXenes exhibit a surface-rich chemistry which provides it unique properties and potential  
13 applications<sup>108</sup>. In MXene synthesis, when the “A” layer is selectively etched from the precursor  
14 MAX phase the interlayer spaces are generated between the MXene layers, where solvent  
15 molecules or functional groups are developed (Figure 2a). These surface terminations on  
16 the MXene surface play an important role in defining the properties of MXenes<sup>109</sup>. The nature of  
17 the surface terminations can be altered during the synthesis of MXenes to tailor the surface  
18 chemistry of MXenes<sup>110</sup>. The layered structure of MXenes, combined with their tunable surface  
19 chemistry and properties, allows various applications in electronics, energy storage, catalysis,  
20 sensing, medicines, and more<sup>111, 112</sup>.

21 MXenes typically possess surface terminations, such as -OH, -O, -Cl, or -F, resulting from the  
22 etching process used to synthesize them. During acidic etching, mainly containing fluoride ions,  
23 MXenes typically exhibit -F and -O/-OH groups (Figure 2b). F terminations can be modulated  
24 by adjusting acid concentrations, while their complete replacement with -O/-OH groups can be  
25 achieved through alkaline treatments using KOH, NaOH, or TBAOH<sup>113 114</sup>. The molten salt  
26 etching (like  $\text{ZnCl}_2$ ) facilitates Lewis acid-base reactions between cations and the A layer,  
27 substituting it with Zn and then followed by -Cl terminations<sup>115</sup>. Variation in the composition of  
28 molten salts during MAX phase etching facilitates the incorporation of halogen terminations, such  
29 as -Cl, -Br, and -I. In addition to these, a wide range of terminations, such as -S, -Se, -Te, -P,  
30 and -Sb, can be uniformly introduced onto MXene surfaces, enabling tailored surface  
functionalities for diverse applications (Fig. 2b). Heating MXenes under reactive gases further



allows the formation of uniform –O and –C terminations. The molten salt method also produces –Cl or –Br terminated MXenes like  $Ti_3C_2Cl_2$ ,  $Nb_2CBr_2$  etc., which can act as templates for post-synthesis modifications, yielding MXenes terminated with –S, –Se, –Te, –NH, –O, or bare/-H groups (Figure 2b).



**Figure 2.** MXenes surface terminations. (a) A schematic representation of the MXene structures, indicating the surface terminations of the outer metal layers. Reproduced with permission from Ref.<sup>111</sup>. Copyrights 2021, The American Association for the Advancement of Science. (b) MXene termination scenarios: (i) Halogen and –O–OH terminations from the acidic etching of MAX phases, (ii) Surface terminations from molten salts, (iii) Surface terminations via molten salts via altered treatment, (iv) Post-synthesis modification introduce uniform terminations. (c) Surface terminations: (i) FCC sites, (ii) "Top" positions on surface Ti, (iii) HCP sites, and (iv) Bridge sites between Ti atoms. Reproduced with permission from Ref.<sup>116</sup>. Copyrights 2023, American Chemical Society.

Theoretical investigations show that MXene surface terminations occupy distinct crystallographic sites<sup>117</sup>. For  $Ti_3C_2T_x$  MXene, terminations above middle Ti atoms align with FCC sites, while those above surface Ti atoms adopt a “top” configuration, and those above C atoms occupy “HCP” sites. Terminations between Ti atoms form a “bridge” configuration (Figure 2c). FCC sites are energetically most favorable among these, with most terminations preferring these positions.

1 These terminations play a significant role in determining the surface chemistry, stability, and  
2 interactions of MXene with other materials<sup>118</sup>. The surface terminations of MXenes offer  
3 opportunities for functionalization<sup>119</sup>. The presence of water-loving polar surface terminations,  
4 particularly -OH groups, leads to a strong affinity for water molecules and promotes wetting of the  
5 MXene surface<sup>119</sup>. This hydrophilicity can be advantageous for applications such as water  
6 treatment and filtration<sup>120</sup>. The surface chemistry of MXenes influences their solubility and  
7 interactions with solvents. MXenes are generally not soluble in common organic solvents but are  
8 dispersible in water-based solutions due to their hydrophilic nature<sup>121</sup>. This solubility behavior  
9 enables their use in solution processing techniques and the fabrication of MXene-based films,  
10 coatings, and composites.

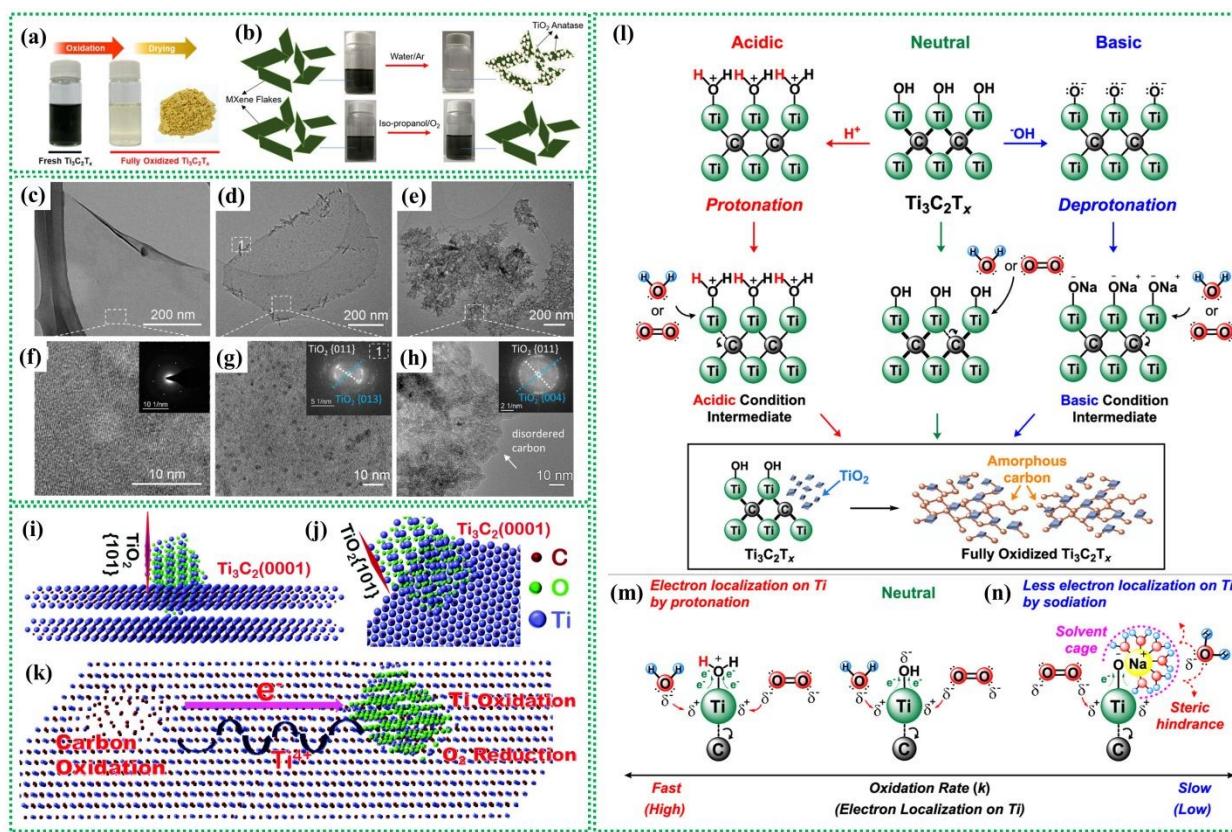
### 11 **3.1 MXenes oxidation and its factors**

12 MXenes oxidize when exposed to ambient conditions or elevated temperatures, transforming into  
13 their corresponding oxides. For example,  $Ti_3C_2T_x$  MXene evolves into a  $Ti_3C_2T_x/TiO_2$  and  
14 eventually forms carbon-supported  $TiO_2$  nanoparticles<sup>122, 123</sup>. It has been reported earlier that the  
15 MXene oxidation starts at the edges of MXene flakes and advances toward the interior basal  
16 planes<sup>124, 125</sup>.

17 The oxidation can be observed through color changes; fresh  $Ti_3C_2T_x$  MXene dispersed in water  
18 has a dark green, which is converted to a translucent, cloudy hue as oxidation progresses with time  
19 (Figure 3a). The MXenes oxidation is relatively faster in aqueous suspensions than in organic  
20 dispersions<sup>108, 126</sup>. MXene hydrolysis is crucial in transforming MXenes into respective oxides in  
21 aqueous suspensions, a process that can be inhibited in organic solvents. For instance, no oxidation  
22 was observed in iso-propanol solutions of MXenes stored under an  $O_2$  atmosphere for a same  
23 duration<sup>126</sup> (Figure 3b). TEM analysis of freshly prepared MXenes shows clean surfaces and edges  
24 (Figure 3c), with high-resolution TEM images revealing single-crystalline nanosheets (Figure  
25 3f)<sup>47</sup>. The SAED pattern confirms a hexagonal atomic structure (Inset: Figure 3f). After one week  
26 of exposure to air at room temperature, MXene edges display "branch-like" features, and  
27 crystalline nanoparticles form on the basal planes of the flakes (Figure 3d, g), identified as anatase  
28 in the fast Fourier transform (FFT). After 30 days, MXenes completely decompose into anatase  
29 clumps and disordered carbon (Figure 3e, h). The presence of dissolved oxygen and water leads to  
30 a reaction with the active edges of the flakes, resulting in  $TiO_2$  formation. MXene oxidation is



influenced by various factors. For example, the chemical etching process used to synthesize MXenes in strong acids creates surface defects in MXene flakes<sup>127, 128</sup>. Under ambient conditions or in aqueous suspension, these defect-rich sites ease oxidative degradation, which in turn impact the properties of MXenes<sup>129</sup>. Environmental factors, such as exposure to air or immersion in water, further contribute to MXene degradation. The stability and reactivity of MXenes are significantly influenced by factors like the pH of the dispersion<sup>130, 131</sup>, storage temperature<sup>131</sup>, MXene concentration<sup>132, 133</sup>, flake size, etc<sup>125, 132</sup>.



**Figure 3.** (a) Digital images of  $\text{Ti}_3\text{C}_2\text{T}_x$  suspensions before and after oxidation. Reproduced with permission from ref.<sup>123</sup>. Copyrights 2021, American Chemical Society. (b) MXene dispersion impact in water and isopropanol. Reproduced with permission from ref.<sup>134</sup>. Copyrights 2019, American Chemical Society. TEM images of (c) MXene flakes of fresh  $\text{Ti}_3\text{C}_2\text{T}_x$  solution and solutions stored at room temperature in the air after (d) 7 days and (e) 30 days. (f-h) HRTEM images corresponding to panels c-e, respectively. In Figure f, the inset shows the corresponding SAED pattern, while Figures g and h display the respective FFT patterns. Reproduced with permission. Reproduced with permission from ref.<sup>47</sup>. Copyright 2017, American Chemical Society. Defects in MXenes: (i)-(j) Depiction of  $\text{TiO}_2$  cluster bonding with  $\text{Ti}_3\text{C}_2$ , highlighting the  $\text{TiO}_2$ -(101) plane-oriented perpendicular to the MXene basal plane (0001). (k) Schematic illustrating  $\text{Ti}_3\text{C}_2$  oxidation, showing carbon oxidation at the positive side and Ti-ion oxidation at the negative side of the internal electric field. Rapid electron transport to the convex area and slow Ti-ion diffusion create the internal electric field. Reproduced with permission from ref.<sup>127</sup>.



Copyright 2022, The Royal Society of Chemistry. Effect of pH on MXenes oxidation: (l) Proposed mechanism for the oxidation reaction in  $Ti_3C_2T_x$  mixtures under (m) Acidic and (n) Basic conditions. Reproduced with permission.<sup>123</sup> Copyright 2021, American Chemical Society.

During sonication-assisted delamination, maintaining a constant temperature and using Ar can prevent oxidation. Storing solutions in Ar-sealed vials or refrigeration reduces oxidation. Using mild etchants like tetraethylammonium hydroxide (TMAOH) avoids fluorine by-products, enhancing the stability of MXenes<sup>135</sup>. MXenes should be protected from UV exposure as prolonged exposure leads to faster oxidation<sup>136</sup>. Synthesis methods determine surface terminations, with HF-etching resulting in more -F terminations compared to those synthesized with LiF-HCl<sup>137</sup>. Etching MAX phases with alkali and molten salts prevents MXenes oxidation and hydrolysis<sup>101, 138</sup>. HF etching introduces defects, accelerating degradation to  $TiO_2$ . Relatively mild acids like HCl/LiF and fluorine-free etchants like TMAOH, NaOH, or KOH reduce the MXene defects. Defects in MXenes also facilitate oxidation. Defects in MXenes, created during etching, drive oxidation and affect reactivity, structural changes, conductivity, and functional group formation<sup>128, 139</sup>. Adjusting etchants concentration can control defects which can also boost the resistance against oxidation as well as the performance in desired applications. In  $Ti_3C_2$  MXene, Ti atoms form  $TiO_2$  nanoparticles while the remaining carbon atoms cluster to produce amorphous carbon, resulting in C@ $TiO_2$  heterojunctions<sup>127</sup>. During oxidation at room temperature, the anatase  $TiO_2$  (101) plane is oriented perpendicular to the  $Ti_3C_2$  basal plane (Figure 3i, j). The rotation of the  $TiO_2$ -(101) lattice plane during nucleation depletes  $Ti^{3+}$  in adjacent  $Ti_3C_2$  crystals, creating Ti vacancies and excess carbon atoms. Ti vacancies are commonly found in the surface layer of MXenes prepared via exfoliation methods. Ti-vacancies in  $Ti_3C_2$  MXenes create an internal electric field that drives electron flow, carbon cluster nucleation, and Ti-cation diffusion. This field enhances carbon oxidation, forming  $TiO_2$  nanoparticles and amorphous carbon. Ti-vacancies also facilitate O<sub>2</sub> entry into the lattice, promoting  $TiO_2$  nucleation and growth. Wrinkles and atomic steps act as nucleation sites for oxidation, with Ti-vacancies promoting carbon oxidation and  $TiO_2$  formation (Figure 3k).

Temperature and pH significantly influence MXene oxidation by affecting its reaction kinetics and pathways<sup>52, 87</sup>. Higher pH slows oxidation at 20 °C, while increased temperature accelerates it. The oxidation mechanism of aqueous  $Ti_3C_2T_x$  MXene dispersions starts at -OH group sites, with pH significantly impacting reaction intermediates (Figure 3l). Acidic conditions protonate surface hydroxyls, enhancing Ti atom electrophilicity and promoting nucleophilic addition reactions with



1 H<sub>2</sub>O or O<sub>2</sub>. In basic conditions, excess OH- deprotonates hydroxyls, form sodiated intermediates  
 2 and bulky solvent cages that hinder oxidation due to steric effects and reduced electrophilicity  
 3 (Figure 3m-n).

#### 4 **4. MXene-polymer hybrids for oxidation prevention**

5 MXene-polymer nanocomposites are increasingly recognized for their ability to prevent MXene  
 6 oxidation, as polymers serve as protective layers that shield MXenes from environmental  
 7 degradation. The polymers can preserve MXenes for more than 180 days<sup>140</sup>. These  
 8 nanocomposites can preserve MXenes not only at room temperature but also under higher  
 9 temperatures and moist conditions<sup>141</sup>. This integration not only enhances the stability of MXenes  
 10 but also improves their overall performance in various applications. Table 1 summarizes some  
 11 MXene-polymer combinations investigated to enhance MXene stability over different periods.

12 **Table 1.** MXene-polymer nanocomposites for MXene stability improvement

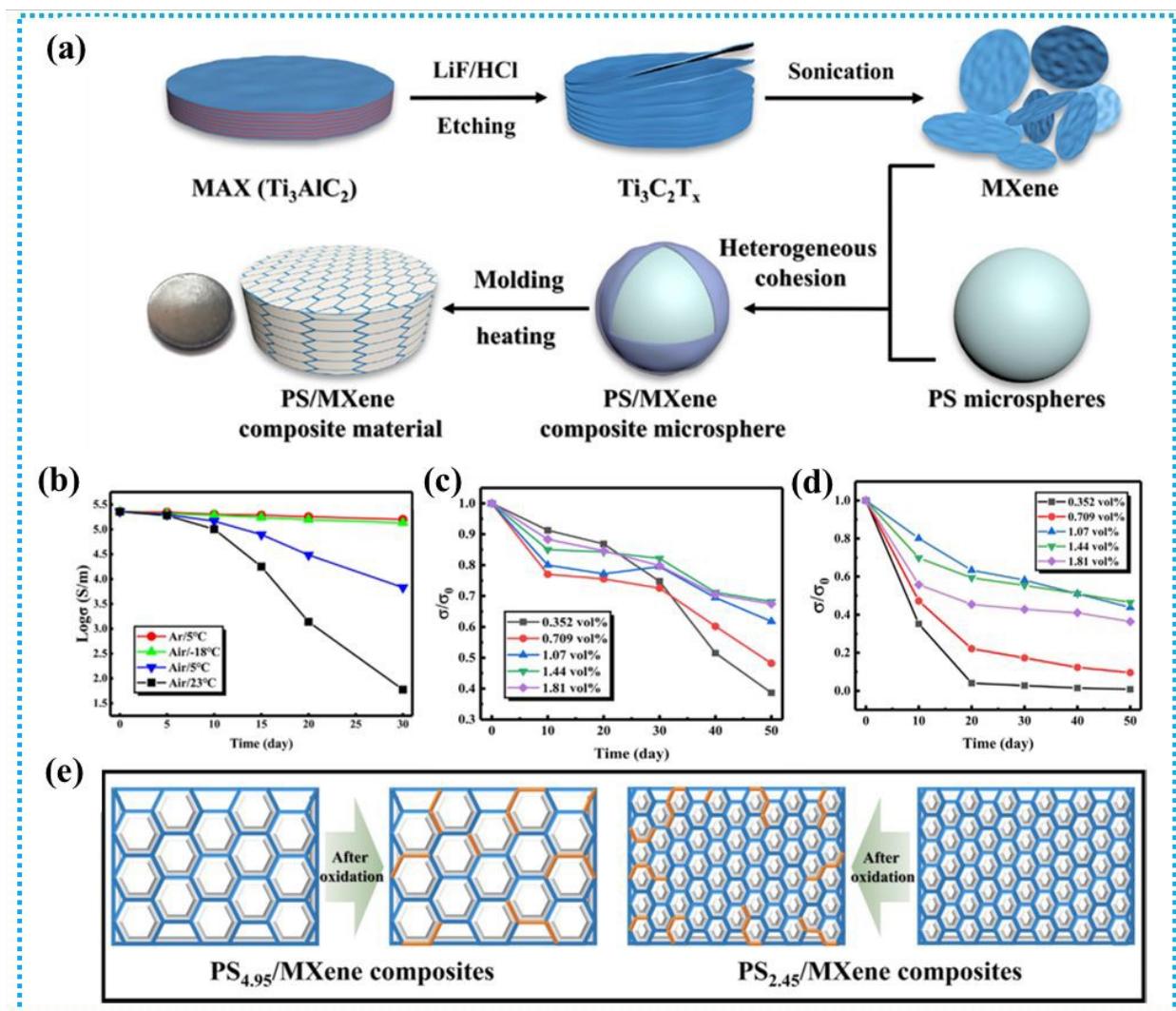
| S. No. | MXene-polymer composition    | MXene etchant | Preventive measure        | Stability duration | Ref.           |
|--------|------------------------------|---------------|---------------------------|--------------------|----------------|
| 1      | MXene/poly(tannic acid)      | LiF/HCl       | Oxygen-rich macromolecule | 60 days            | <sup>142</sup> |
| 2      | MXene/melamine               | LiF/HCl       | Nanocomposite             | 60 days            | <sup>143</sup> |
| 3      | MXene/PVA-CA hydrogel        | LiF/HCl       | Nanocomposite             | 30 days            | <sup>144</sup> |
| 4      | MXene/polymer                | -             | Nanocomposite             | 42 days            | <sup>145</sup> |
| 5      | MXene/polyacrylamide         | -             | Nanocomposite             | 15 days            | <sup>146</sup> |
| 6      | MXene/aramid nanofiber (ANF) | LiF/HCl       | Nanocomposite             | -                  | <sup>147</sup> |
| 7      | MXene/polystyrene            | LiF/HCl       | Nanocomposite             | 180 days           | <sup>140</sup> |
| 8      | MXene/dopamine               | LiF/HCl       | Nanocomposite             | 13 hours at 170 °C | <sup>148</sup> |
| 9      | MXene/Bentonite              | LiF/HCl       | Nanocomposite             | 2 hours at 600 °C  | <sup>149</sup> |
| 10     | MXene/Sodium alginate        | LiF/HCl       | Nanocomposite             | 30 days            | <sup>150</sup> |
| 11     | MXene/PVA                    | LiF/HCl       | Nanocomposite             | 50 days            | <sup>151</sup> |
| 12     | MXene/PET                    | LiF/HCl       | Nanocomposite             | 200 hours at 70 °C | <sup>141</sup> |
| 13     | MXene/polymer                | LiF/HCl       | Nanocomposite             | 180 days           | <sup>152</sup> |

#### 13 **4.1 Polystyrene/MXene for oxidation improvement**

14 To address the issue of MXene oxidation, a '*particle manufacturing technique*' (Figure 4a) was  
 15 employed to develop polystyrene/MXene (PS/MXene) composites with a 3D conductive network  
 16 structure<sup>140</sup>. The material conductivity reached 3846.15 S/m when the filler content was merely



1 1.81 vol%. Due to the compact and ordered structure of fabricated PS/MXene composite, it holds  
 2 53.4% of its initial conductivity after 180 days.



3  
 4 **Figure 4.** (a) Schematic showing the exfoliation of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene and fabrication of composites  
 5 with a three-dimensional conductive network framework. (b) Storage environment effects on  
 6 MXene's intrinsic conductivity. (c-d) Impact of environmental factors on conductivity during the  
 7 composite material is being prepared, and (e) Schematic of the oxidation mechanism in MXene-  
 8 polymer composite. Reproduced with permission from ref.<sup>140</sup>. Copyright 2021, Elsevier Ltd.

9 The fundamental procedure for exfoliating  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene and creating PS/MXene composites  
 10 with a 3D ordered structure through "particle construction".<sup>153</sup> Firstly, this work used the  
 11 conventional technique of manufacturing MXene because of its benefits, which include large  
 12 lamellae, fewer flaws, and good electrical conductivity when created by LiF/HCl etching<sup>154</sup>. The  
 13 electrical conductivity of freshly prepared MXene sheets was initially measured at  $2.28 \times 10^5 \text{ S/m}$ ,  
 14 as shown in Figure 4b. This conductivity remained stable over 30 days in an argon atmosphere or



1 at low temperatures. However, in the air at room temperature, MXene's conductivity dropped  
2 drastically, retaining only 0.026% of its initial value, highlighting its rapid oxidation and reduced  
3 practicality. The interaction between conductivity and storage time for PS/MXene composites is  
4 illustrated in Figure 4c-d. Key findings include: (1) Composites with higher MXene content  
5 maintain conductivity better over time compared to those with lower MXene content, showing  
6 slower degradation. (2) Larger particle composites exhibit greater conductivity loss than those with  
7 smaller particles, regardless of MXene concentration. Additionally, smaller PS microspheres  
8 create a denser conductive network, providing superior protection for MXene, as depicted in  
9 Figure 4e. At larger microspheres, the conductive network is not well established while smaller  
10 microspheres can form a much denser network, that certainly offers superior MXene protection.

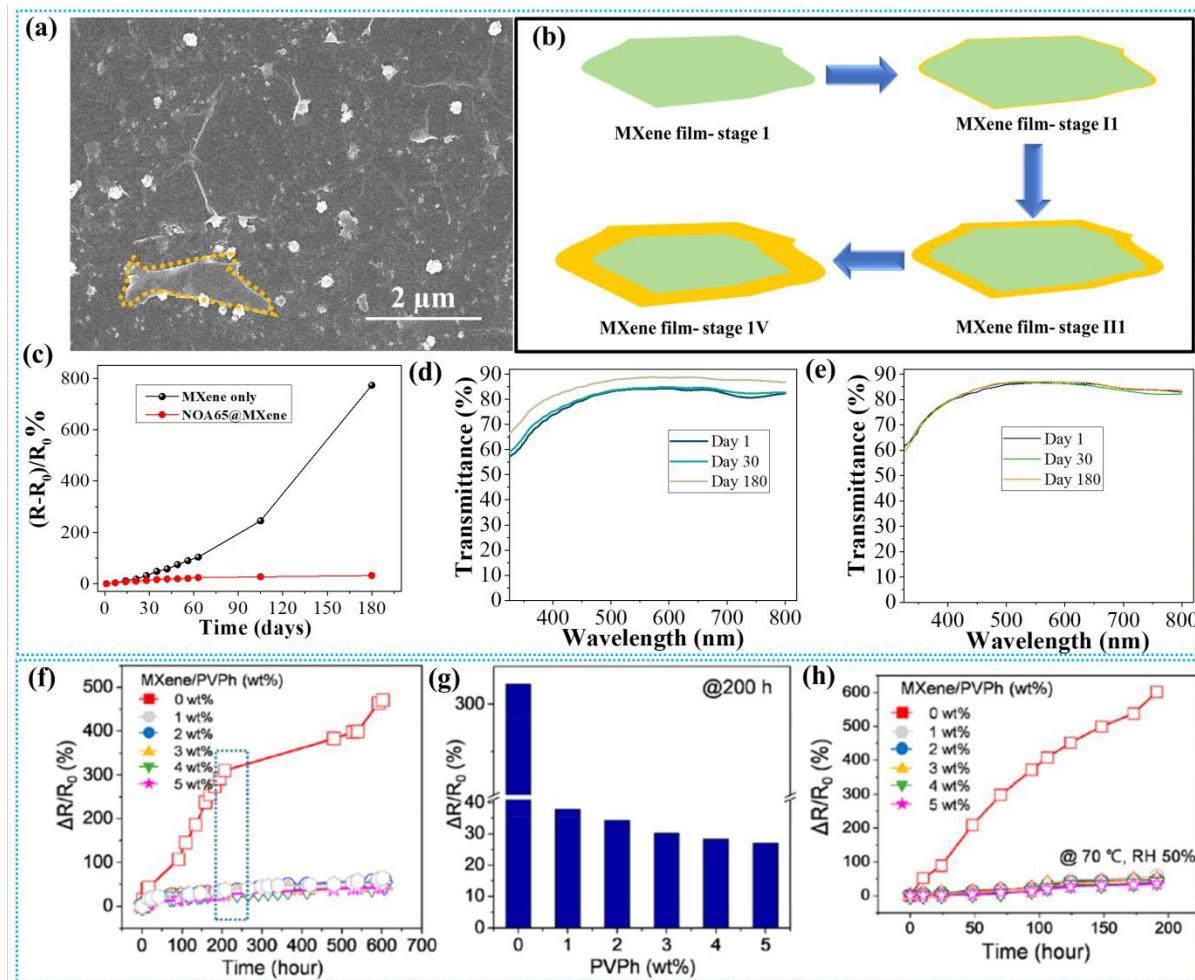
## 11 **4.2 Polymer passivation**

12 Polymer passivation is a technique used to improve the oxidation stability of MXenes, particularly  
13 against oxidation. By applying a polymer coating, such as polydopamine, the surface of MXenes  
14 is protected from environmental factors that can lead to degradation. This passivation method  
15 effectively reduces the oxidation rate and maintains the electrical properties of MXenes over  
16 time<sup>152</sup>. Under ambient conditions, pristine MXene begins to oxidize at room temperature. FE-  
17 SEM images of untreated MXene after 30 days (Figure 5a) reveal powdery particles around the  
18 edges, indicating early oxidation. This process starts at edges and imperfections, progressing  
19 inward as shown in Figure 5b, where oxidized TiO<sub>2</sub> (orange) replaces the MXene flakes (greenish).  
20 Prior reports have indicated that the smaller the MXene flake, the higher the oxidation rate  
21<sup>155</sup>. Even in its dry state, MXene will eventually oxidize, nevertheless, the rate of oxidation is  
22 slower under ambient circumstances than in humid environments or DI water<sup>151</sup>. To prevent  
23 oxidation, a MXene film was coated with a 1% polymer solution in acetone. The polymer layer  
24 thickness was ~50 nm. Sheet resistance (R) was measured over 180 days to evaluate oxidation  
25 stability, with percentage changes (Figure 5c). The results showed obvious proof that polymer  
26 passivation preserves MXene from oxidization. Even 180 days later, the relative resistance change,  
27 (R-R<sub>0</sub>/R<sub>0</sub>)%, is ~20% in polymer-passivated MXene as compared to 800% in pristine MXene. The  
28 UV–Vis spectra of pristine MXene film after 30 days show the same transmittance as on day 1,  
29 however, the transmittance rises to ~89% after 180 days (Figure 5d). The high transmittance may  
30 be associated with TiO<sub>2</sub> formation due to the oxidized Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene<sup>151</sup>. Contrary to this, a  
31 negligible change in transmittance was noticed in the passivated MXene film 180 days (Figure



1 5e), indicating that almost no  $\text{TiO}_2$  is formed and MXene oxidation is suppressed due to polymer  
2 passivation.

3 In another study, a polymer laminated MXene (PL-MXene) electrode was fabricated to analyze  
4 the impact of polymer lamination on electronic applications<sup>141</sup>. MXene flakes dispersed in water  
5 were spin-coated on a glass substrate silanized with a self-assembled monolayer of (3-  
6 aminopropyl)triethoxysilane (APTES).



7  
8 **Figure 5.** MXene passivation by polymers. (a) FE-SEM image of MXene sheet after 30 days  
9 exposure in ambient circumstances. The MXene flake that has been highlighted indicates the start  
10 of oxidation, (b) An illustration of the oxidation phases of MXene flakes. (c) The ratio of resistance  
11 change ( $R - R_0/R_0\%$ ) for treated and non-treated MXene films up to 180 days, where  $R_0$  is the initial  
12 sheet resistance. UV-Vis spectra of MXene films (d) non-treated and (e) treated at varying times.  
13 Reproduced with permission from ref.<sup>152</sup>. Copyright 2022, Elsevier Ltd. (f) PL-MXene electrode's  
14 oxidation stability in comparison to the thin MXene layer. (g) The resistance decrease ( $\Delta R$ ) and  
15 initial resistance ( $R_0$ ) of the PL-MXene electrode are shown against time and PVPh concentration,  
16 200 hours after exposure to air oxidation, (h) Evolution of the resistance variations over time of



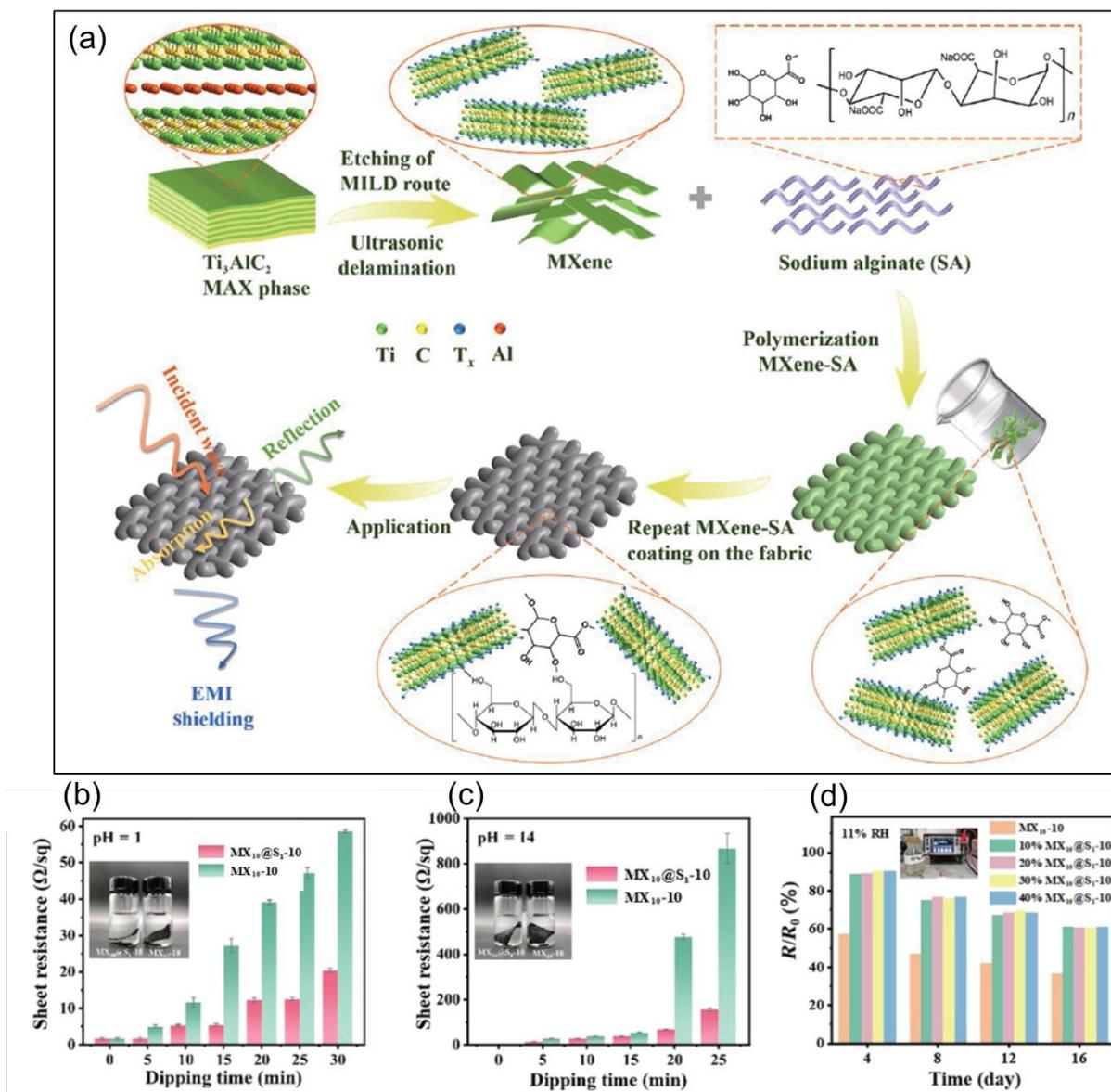
1 the PL-MXene electrode under oxidation stability tests at 50% humidity and 70 °C. Reproduced  
2 with permission from ref.<sup>141</sup>. Copyright 2021, American Chemical Society.

3 Subsequently, poly(4-vinyl phenol) (PVPh) was prepared as a barrier layer on the MXene film<sup>141</sup>.  
4 The PL-MXene film, coated with a PVPh layer (~60 nm) on an MXene layer (~18 nm), exhibits a  
5 very smooth surface with an RMS roughness of ~1.4 nm. After 200-600 hours of air exposure, the  
6 resistance of bare MXene increases by 310% and 470%, respectively (Figure 5f). In contrast, PL-  
7 MXenes with PVPh coatings showed minimal resistance change, between 27% and 38% after 200  
8 hours, with only slight increases after 600 hours, demonstrating excellent oxidation resistance  
9 (Figure 5g). Even at 70 °C temperature and 50% relative humidity, PL-MXenes with PVPh  
10 coatings maintained good stability, showing a  $\Delta R/R_0$  change of 35% to 60% after 200 hours, while  
11 bare MXene showed a drastic increase to 600% (Figure 5h).

#### 12 **4.3 MXene-sodium alginate nanocomposites**

13 Sodium alginate (SA) effectively stabilizes MXenes against oxidation. The alginate-stabilized  
14 MXenes maintain their conductivity and offer improved oxidation resistance. These MXene-  
15 alginate nanocomposites are particularly useful in flexible EMI shielding applications. Figure 6(a)  
16 shows the schematic illustrating the fabrication process of the MXene-SA composite<sup>150</sup>. Linen  
17 fabric, chosen for its eco-friendly properties, was used as a substrate for MXene composite  
18 modification. Before applying the composite, the fabric was treated with decontamination powder  
19 to ensure effective loading. Hydrogen bonding between SA and MXene was achieved via  
20 functional groups on the MXene surface, enhancing the composite's mechanical strength and  
21 oxidation stability. MXene-SA composites and MXene alone were subjected to acid and base  
22 conditions to assess environmental stability and oxidation resistance. After 30 minutes in HCl (pH  
23 = 1), the sheet resistance of MX10@S<sub>1</sub>-10 (MXene with SA) increased to  $20.4 \pm 0.7 \Omega/\text{sq}$ , whereas  
24 MX10-10 (MXene without SA) showed a much higher increase to  $58.63 \pm 0.047 \Omega/\text{sq}$  (Figure 6b).  
25 In NaOH (pH = 14), MX10@S<sub>1</sub>-10's resistance rose to  $155.33 \pm 7.02 \Omega/\text{sq}$  after 25 minutes,  
26 compared to a significant rise to  $867.67 \pm 66.38 \Omega/\text{sq}$  for MX10-10 (Figure 6c). This demonstrates  
27 that the MXene-SA composite offers superior protection against oxidation in both acidic and basic  
28 environments. The results manifest that MX<sub>10</sub>@S<sub>1</sub>-10 has much better stability than MX<sub>10</sub>-10 even  
29 in harsh conditions such as acidic and alkaline. The coating of MXene sheets with SA inhibited  
30 the direct interaction of ambient oxygen, moisture, or corrosive solutions resulting in improved  
31 oxidation stability.





**Figure 6.** (a) Schematic synthesis of MXene and illustration for single-step fabrication strategy for sodium alginate-MXene film, Sheet-resistance ( $R/R_0$ ) variation by treating in (b) HCl ( $\text{pH} = 1$ ), (c) NaOH ( $\text{pH} = 14$ ), and (d) change in  $R / R_0$  for  $\text{MX}_{10}-10$  and  $\text{MX}_{10}@\text{S}_1-10$  with varying SA content at 11% of RH at  $25^\circ\text{C}$ . Reproduced with permission from ref.<sup>150</sup>. Copyright 2024, Springer Nature.

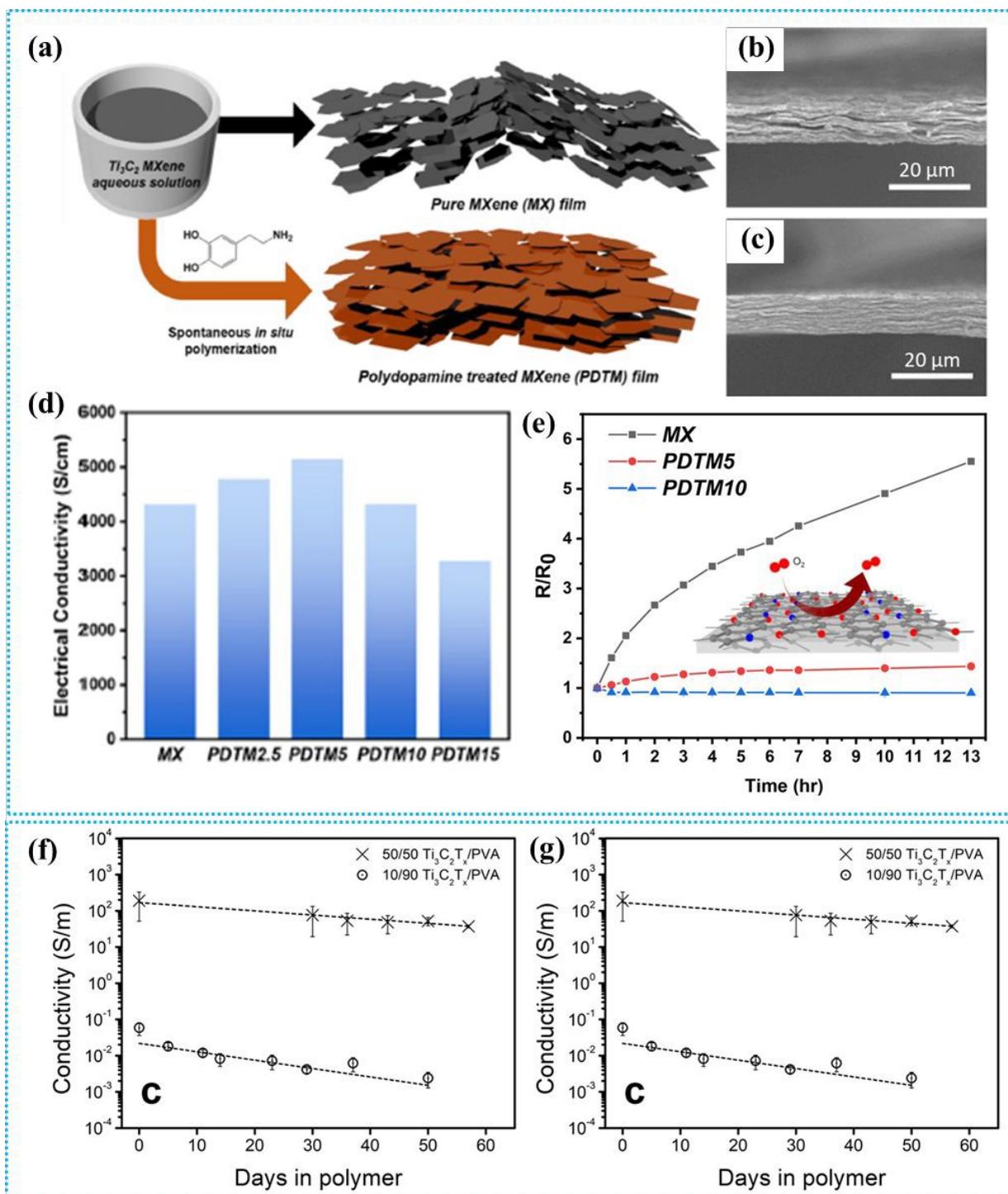
The oxidation stability of fabricated MXene composites was further studied by measuring their sheet resistance after storing in humid conditions at ambient temperature ( $25^\circ\text{C}$ ).  $\text{MX}_{10}-10$  and  $\text{MX}_{10}@\text{S}_1-10$  were stored in humid conditions (RH) of 11%, 33%, 75.5%, and 97.6% with varied SA amounts of 10%, 20%, 30%, and 40% for evaluating the stability. There is a change in resistance of  $\text{MX}_{10}-10$  composite with time at 11% RH ambient, with the resistance ratio decreasing to 36.67% from 57.48%. The resistance ratio decreased from 88.56% to 60.99% for

1 MX<sub>10</sub>@S<sub>1</sub>-10 upon the 10% addition of SA (Figure 6d). MX<sub>10</sub>@S<sub>1</sub>-10 has a higher resistance ratio  
2 than MX<sub>10</sub>-10 indicating that MX<sub>10</sub>@S<sub>1</sub>-10 has a higher stability under varied humid and corrosive  
3 conditions.

#### 4 **4.4 Mussels-derived dopamine polymerization**

5 Researchers addressed the oxidation vulnerability of MXene-based materials by utilizing mussel-  
6 derived dopamine polymerization<sup>148</sup>. Dopamine derived from mussels effectively overcomes  
7 oxidation by enhancing interfacial interaction and ordering in MXene film. Dopamine forms a thin  
8 sticky layer at the surfaces of MXene flake by in situ polymerization and binding caused by  
9 spontaneous interfacial charge transfer. Effective oxygen and moisture screening also significantly  
10 increases the ambient stability of MXene films. It's interesting to note that angstrom thick  
11 polydopamine enhances MXene films' inherent high electrical conductivity. Figure 7a shows the  
12 fabrication procedure and morphological distinction between pure- and polydopamine-treated  
13 MXene (PDTM) film. SEM cross-sectional images show that pure MXene has random, misaligned  
14 layers, while PDTM5 films exhibit well-aligned, consistent MXene sheets (Figure 57b, c).  
15 Neighboring MXene flakes are aligned in their organized stacking by the polydopamine nano  
16 binder, which bridges them together and creates the highly ordered MXene structure<sup>156</sup>. After  
17 applying polydopamine coating, internal voids, and misfits could be mostly eliminated<sup>157</sup>. As a  
18 result, dopamine coating increased the apparent density of hybrid films resulting in in-plane  
19 electron transfer. Furthermore, dopamine hybridization enhances MXene's electrical conductivity;  
20 PDTM5 has the greatest conductivity of 5141 S/cm Figure 7d. The enhanced flake alignment,  
21 enhanced film densification, and increased electron density all contribute to in-plane electron  
22 transport<sup>158</sup>. Polydopamine-treated MXene films exhibit significantly reduced oxidation at  
23 ambient conditions and elevated temperatures, as shown in Figure 7(e). The PDTM5 film  
24 experiences a much smaller increase in sheet resistance at 170°C compared to the pure MXene  
25 film, which shows a five-fold resistance increase in 13 hours. The PDTM10 film demonstrates  
26 even lower resistance, likely due to thermally induced crystallization of the polydopamine layer,  
27 which also limits oxygen and moisture infiltration.





**Figure 7.** (a) Schematic showing the production process and the morphological changes between pure and polydopamine-treated MXene film, (b) and (c) Cross-sectional SEM images of pure- and PDTM-treated MXene, (d) electrical conductivity of MXene film with varied PDTM concentration (0-15%), (e) Change in electrical resistance during heating (170 °C) in air. Reproduced with permission from ref.<sup>148</sup>. Copyright 2020, American Chemical Society. The conductivity variation of (f) Pristine MXene films and (g) MXene/PVA films in air<sup>151</sup>.





1  
2 The thin dopamine layer protects MXene from oxidation while maintaining electrical performance  
3 and enhancing interfacial contact.

#### 4 **4.5 Can all polymers prevent MXene oxidation?**

5 As discussed above, while most polymers support MXene stability, not all polymers can  
6 effectively prevent oxidation. Polymers with a hydrophilic nature are mostly unable to prevent  
7 oxidation in MXenes as hydrophilicity allows water and oxygen molecules to penetrate the  
8 composite and the MXene surface. Habib et al. studied the oxidation stability of vacuum-filtered  
9  $Ti_3C_2T_x$  films MXenes/PVA films and used the electrical conductivity as an indicator to estimate  
10 their stability<sup>151</sup>. The study monitored the decline in electrical conductivity of  $Ti_3C_2T_x$ /PVA  
11 composites over time and compared it with pristine MXene films exposed to air (Figure 7f-g). Two  
12 different weight ratios of PVA were used to assess the impact of polymer concentration on the  
13 stability of MXenes: 50–50 wt%  $Ti_3C_2T_x$  to PVA and 10–90 wt%  $Ti_3C_2T_x$  to PVA. The study  
14 reported that the pristine MXene maintained only 2% of its initial conductivity in air after 9 weeks  
15 (Figure 7f). The conductivity of the 50–50 wt% sample decreased to about 40% of its original  
16 value by day 30 and 20% by day 57, while the 10–90 wt% sample dropped to roughly 7% by day  
17 29 and 4% by day 50 (Figure 7g). Both samples exhibited a rapid decline in conductivity during  
18 the first four weeks, followed by a slower decrease, indicating a reduction in oxidation rates due  
19 to diminishing reactive sites. This consistent trend across both composite samples and the  $Ti_3C_2T_x$   
20 film suggests that the oxidation mechanism is mostly unaffected by polymer content, and the  
21 hydrophilic PVA does not provide an effective protective barrier against oxidation.

### 22 **5. Synergistic effects on nanocomposite properties**

23 Typically, the main benefit of composite membranes lies in their tailored properties, allowing the  
24 use of specific materials for particular applications. MXene materials can serve as optimal  
25 nanofillers, enhancing MXene/polymer membranes with a range of properties such as increased  
26 mechanical strength<sup>159</sup>, better thermal performance<sup>160</sup>, and enhanced conductivity<sup>161</sup>, etc.  
27 Moreover, the oxidation of MXene materials is significantly reduced due to their effective  
28 encapsulation within the polymer<sup>162</sup>. MXenes can be combined with two types of polymers:  
29 cationic and neutral<sup>163</sup>. The cationic polymer (e.g. PDDA) can form electrostatic interactions with  
30 negatively charged MXene nanosheets, resulting in a relatively loose structure with some voids,  
31 similar to the MXene-only film. In contrast, the neutral polymer (e.g. PVA) can rely on hydrogen

1 bonding, leading to a compact layered structure (Figure 8a). Using negatively charged polymers  
2 can enhance the dispersion of MXene nanosheets due to electrostatic repulsion. Molecular  
3 dynamics simulations reveal the synergy of hydrogen and ionic bonding agents in effectively  
4 transferring local stress while providing substantial slippage space for MXene nanosheets<sup>164</sup>.

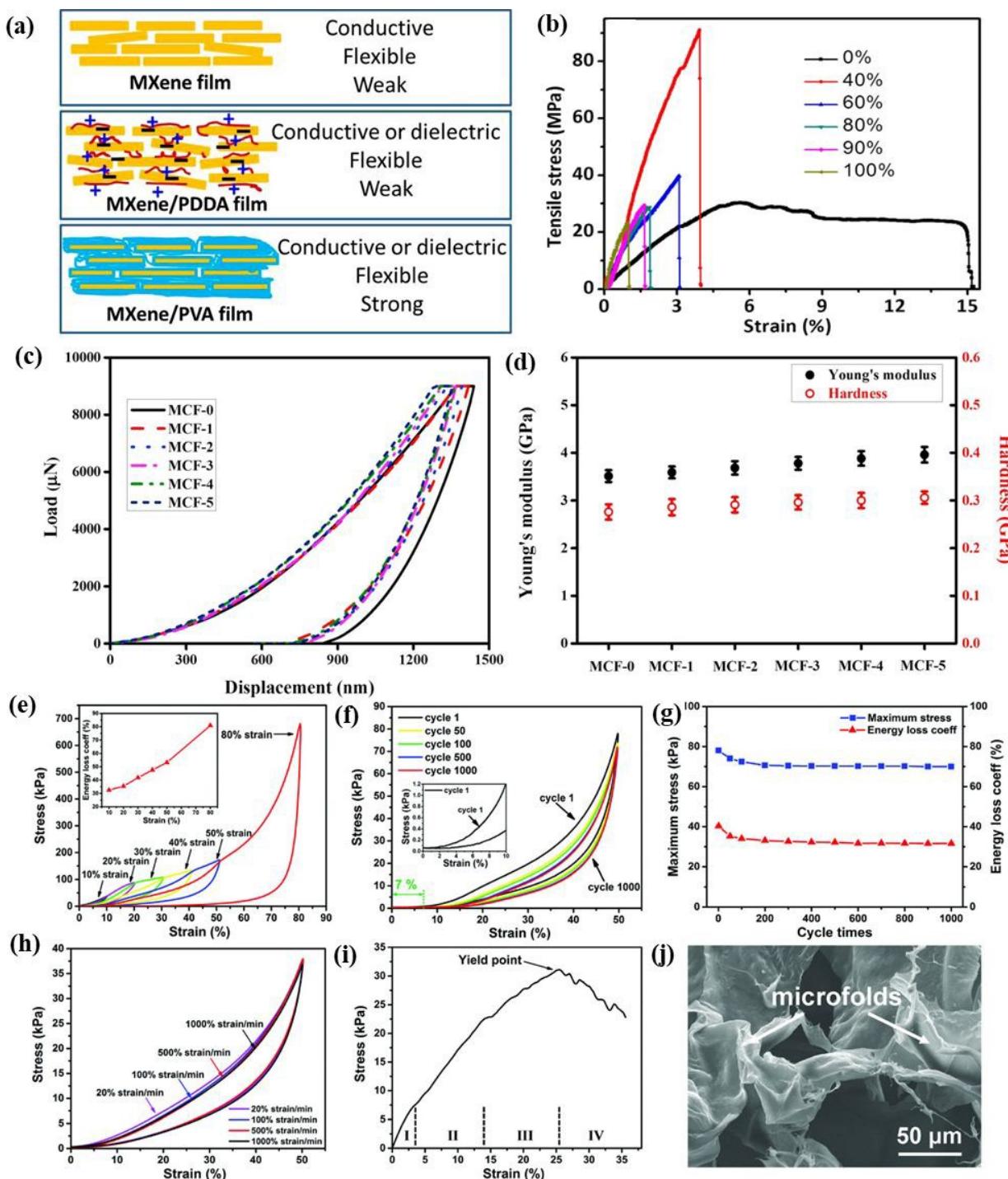
### 5 **5.1 Mechanical properties**

6 The mechanical properties represent a crucial factor for polymer-based composites, which can be  
7 effectively enhanced by incorporating inorganic fillers. The distinctive characteristics and  
8 nanostructures of nanomaterials, along with their reactivity, have made them appealing candidates  
9 as fillers to strengthen polymer-based membranes across various types of polymers. Usually, free-  
10 standing MXenes often experience inadequate mechanical characteristics and weak interactions  
11 among the nanosheets, which can lead to structural failure due to capillary forces during the  
12 polymer impregnation process. Introducing 10 wt% PVA improves the tensile strength of the  
13  $Ti_3C_2T_x/PVA$  film by 34%, reaching  $91 \pm 10$  MPa, around fourfold that of the pure  $Ti_3C_2T_x$  film,  
14 when PVA loading was increased to 60 wt%<sup>163</sup> (Figure 8b). The enhanced stiffness and strength  
15 indicate effective stress transfer to the embedded  $Ti_3C_2T_x$  nanosheets, suggesting some interfacial  
16 bonding, likely aided by the OH group terminations on  $Ti_3C_2T_x$ . The Young's modulus of  
17  $Ti_3C_2T_x/PVA$  films can be adjusted by varying the  $Ti_3C_2T_x$ -to-PVA ratio. The hollow cylinders  
18 made from these films can support substantial weights, with a 6 mm diameter and 10 mm high  
19 cylinder supporting about 4,000 times its weight ( $\sim 1.3$  MPa), and a similar cylinder with 90 wt%  
20  $Ti_3C_2T_x/PVA$  supporting approximately 15,000 times its weight ( $\sim 2.9$  MPa).

21 To explore this issue in greater depth, researchers have created MXene composite frameworks by  
22 adding crosslinking agents to connect MXene nanosheets. Researchers combined resorcinol and  
23 formaldehyde with  $Ti_3C_2T_x$  to form a composite framework<sup>165</sup>. The organic precursors  
24 polymerized on hydrophilic  $Ti_3C_2T_x$ , creating a crosslinked  $Ti_3C_2T_x/C$  foam (MCF) structure after  
25 pyrolysis. This framework exhibited a well-connected structure with impressive mechanical  
26 strength, supporting 500 times its weight. Using a similar polymer impregnation method with  
27 epoxy precursors, a dense  $Ti_3C_2T_x/C$ /epoxy film structure was also produced. The MCF samples  
28 were labeled as MCF-0 to MCF-5, with increasing  $Ti_3C_2T_x$  MXene content from 0 to 1.64 wt%,  
29 respectively. The SEM images show that adding  $Ti_3C_2T_x$  MXene to the MCF resulted in a



- 1 reduction of cell density due to crosslinked, folded sheets, while further MXene addition increased  
 2 cell density and decreased sheet size.



3  
 4 **Figure 8.** Mechanical properties of MXene-polymer nanocomposite. (a) Schematic representation  
 5 of MXene-based functional films demonstrating tunable mechanical characteristics of flexible,  
 6 free-standing Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>, Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/PVA, and Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/PDDA films. (b) Stress–strain curves  
 7 illustrating the performance of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/PVA films with varying Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> content<sup>163</sup>. (c) Load-

displacement curves showcasing the performance of the MCF/epoxy EMI shielding nanocomposites; (d) Hardness and Young's modulus measurements for the MCF/epoxy EMI shielding nanocomposites, illustrating their mechanical properties. Reproduced with permission from ref.<sup>165</sup>. Copyright 2019, Elsevier Ltd. (e) Compressive stress-strain ( $\sigma$ - $\epsilon$ ) curves for the aerogel (MXene to PAA ratio 1:4) at various strains, with an inset showing energy loss coefficients at these strains. (f) Fatigue performance of the aerogel (MXene to PAA ratio 1:1) subjected to 1000 cycles at 50% strain. (g) Changes in elastic stress and energy loss coefficients over 1000 cycles at 50% strain. (h) Stress-strain curves of the aerogel (MXene to PAA ratio 2:1) evaluated at different compressive strain rates (20, 100, 500, and 1000% min<sup>-1</sup>). (i) Tensile stress-strain curve for the aerogel (MXene to PAA ratio 2:1); (j) SEM image illustrating the fracture morphology of the MXene/PI aerogel. Reproduced with permission from ref.<sup>166</sup>. Copyright 2018, Wiley.

The polymerization of resorcinol and formaldehyde on hydrophilic  $Ti_3C_2T_x$  MXene effectively fused the carbon structure and MXene, enhancing crosslinking density and carbon junctions. The load-displacement curves (Figure 8c) show that increasing  $Ti_3C_2T_x$  MXene content reduces the indentation depth of MCF/epoxy EMI shielding nanocomposites, enhancing their resistance to indentation. As  $Ti_3C_2T_x$  MXene content increases, Young's modulus and hardness improve by 13% and 11%, respectively, due to the superior mechanical properties of MXenes and the improved stress transfer within the cross-linked MCF network (Figure 8d). The higher cell density from additional MXene further strengthens the cross-linked structure, boosting the mechanical performance of the nanocomposites. Liu et al. improved the flexibility and mechanical stability of  $Ti_3C_2T_x$ /PI foam by using polyimide (PI) to bridge  $Ti_3C_2T_x$  nanosheets, achieving compressibility and stretchability through freeze-drying  $Ti_3C_2T_x$ /poly(amic acid) (PAA) followed by polymerization<sup>166</sup>. An aqueous solution of hydrophilic PAA and  $Ti_3C_2T_x$  was freeze-dried, followed by thermal annealing to polymerize PAA into PI. Strong polar interactions between PI and  $Ti_3C_2T_x$  tightly bonded the two components, resulting in a durable  $Ti_3C_2T_x$ /PI foam with excellent mechanical properties, including compression, torsion, and 180° bending. The MXene/PI aerogel demonstrates strong interfacial bonding between MXene and PI, resulting in superior mechanical properties compared to neat MXene aerogel. Figure 8e shows the compressive stress-strain curves, where the MXene/PI aerogel exhibits excellent reversible compressibility up to 80% strain (MXene to PAA ratio 1:4), unlike the pristine MXene aerogel, which suffers from irreversible deformation due to weak interactions between its layers. The MXene/PI aerogel also has a high energy loss coefficient ( $\eta$ ), reaching 80.9% at 80% strain, indicating strong energy absorption. This makes it highly effective for shock absorption, as demonstrated by its ability to protect a glass plate from fracturing after a heavy impact while maintaining its original shape. The



MXene/PI aerogel was tested for fatigue resistance through long-term compression-release cycles. After pre-stabilizing the aerogel with several loading-unloading cycles, it maintained over 90% of maximum stress and only 7% volume deformation after 1000 cycles at a fixed strain of 50% (Figure 8f), indicating excellent structural robustness. While the maximum stress and energy loss coefficient slightly decreased during initial cycles, they stabilized over 1000 cycles (Figure 8g). Additionally, the aerogel retained its compressibility at various strain rates (20, 100, 500, and 1000% min<sup>-1</sup>), with stress-strain curves showing close overlap (Figure 8h). Uniaxial tensile tests show that the MXene/PI aerogel achieves a tensile strain of 26% and a maximum stress of 31.1 kPa, attributed to enhanced sheet-to-sheet interactions with PI (Figure 8i). The tensile stress-strain curve consists of four stages: (1) elastic deformation, where stress increases linearly with strain; (2) densification, marked by continuous stress increase as the porous network compacts; (3) a plateau region with slower stress increases due to friction and adhesion; and (4) fracture, characterized by decreasing stress with fluctuations, indicating structural failure. Fractured surfaces with pleated cell walls illustrate the role of micro folds in tolerating cyclic tensile deformation (Figure 8j). Some of the mechanical properties of MXene-polymer nanocomposites are summarized in Table 2.

**Table 2. Mechanical properties of MXene-polymer nanocomposites**

| S. No. | Polymer                          | MXene   | MXene Concentration   | Mechanical property (MPa) | Improvement percentage (%) | Ref.           |
|--------|----------------------------------|---|---|---------------------------|----------------------------|----------------|
| 1      | Natural rubber                   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 6.71 vol. %   | ~ 18 (tensile stress)     | 700                        | <sup>167</sup> |
| 2      | Epoxy resin                      | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 1.0 wt.%  | 98 (flexural strength)    | 66                         | <sup>168</sup> |
| 3      | PEDOT:PSS                        | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> : polymer (3:1) | 30.18 (tensile strength)  | 503.6                      | <sup>169</sup> |
| 4      | Polyvinyl alcohol (PVA)          | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 2 wt.%  | ~ 48 (tensile stress)     | 77.8                       | <sup>170</sup> |
| 5      | Polyurethane (PU)                | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 0.5 wt.%  | ~ 18 (tensile strength)   | 20                         | <sup>171</sup> |
| 6      | Thermoplastic polyurethane (TPU) | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 0.5 wt.%  | 20.6 (tensile strength)   | 47.1                       | <sup>172</sup> |
| 7      | PVC                              | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 15 wt.%   | 57.3 (tensile strength)   | 174.1                      | <sup>173</sup> |
| 8      | PVA                              | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 0.5 wt.%  | 13 (tensile strength)     | -                          | <sup>174</sup> |



|    |               |   |           |                               |       |     |
|----|---------------|---|-----------|-------------------------------|-------|-----|
| 9  | Epoxy         | Ti <sub>3</sub> CN                            | 90 wt.%   | 12.8 GPa<br>(Young's modulus) | -     | 175 |
| 10 | Epoxy         | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 15 wt.%   | 4.32 GPa<br>(Young's modulus) | 20.8  | 176 |
| 11 | Epoxy         | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 4.25 wt.% | 3.96 GPa<br>(Young's modulus) | 13    | 165 |
| 12 | Polypropylene | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 2.0 wt.%  | 18.4 (tensile strength)       | 35.3  | 177 |
| 13 | PVA           | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 40        | 91 (tensile strength)         | 313.6 | 163 |

1  
 2 **5.2 Electrical properties**  
 3 In any device application, conductivity is a crucial property, and MXenes excel in this regard,  
 4 achieving an impressive electrical conductivity of  $\sim 24,000$  S/cm.<sup>178</sup> Among the MXenes, Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>  
 5 stands as a pinnacle, characterized by its exceptional electrical conductivity and multifaceted  
 6 utility across diverse applications. Most polymers are insulators, but adding MXene flakes can  
 7 improve their electrical conductivity. The addition of MXenes to the polymers can separate the  
 8 layers of MXenes and promote bonding at the molecular level between MXene and the polymer.  
 9 It was found that found that the electrical conductivity of PVA increases from 0.04 to  $2.2 \times 10^4$   
 10 S/m when the MXene (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>) content varies from 40 wt% to 90 wt% in the polymer matrix<sup>163</sup>.  
 11 The relationship between the MXene content in polymer matrix e.g. polyacrylamide (PAM) and  
 12 electrical conductivity is expressed as<sup>179</sup>:

$$13 \quad \sigma = k(m - m_{th})^\alpha$$

14 In this equation,  $\sigma$  represents the electrical conductivity of nanocomposite (Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/PAM)  
 15 membranes,  $k$  is a constant,  $m$  denotes the MXene loading amount,  $m_{th}$  is the percolation threshold  
 16 required for conductivity enhancement, and  $\alpha$  is the scaling exponent.

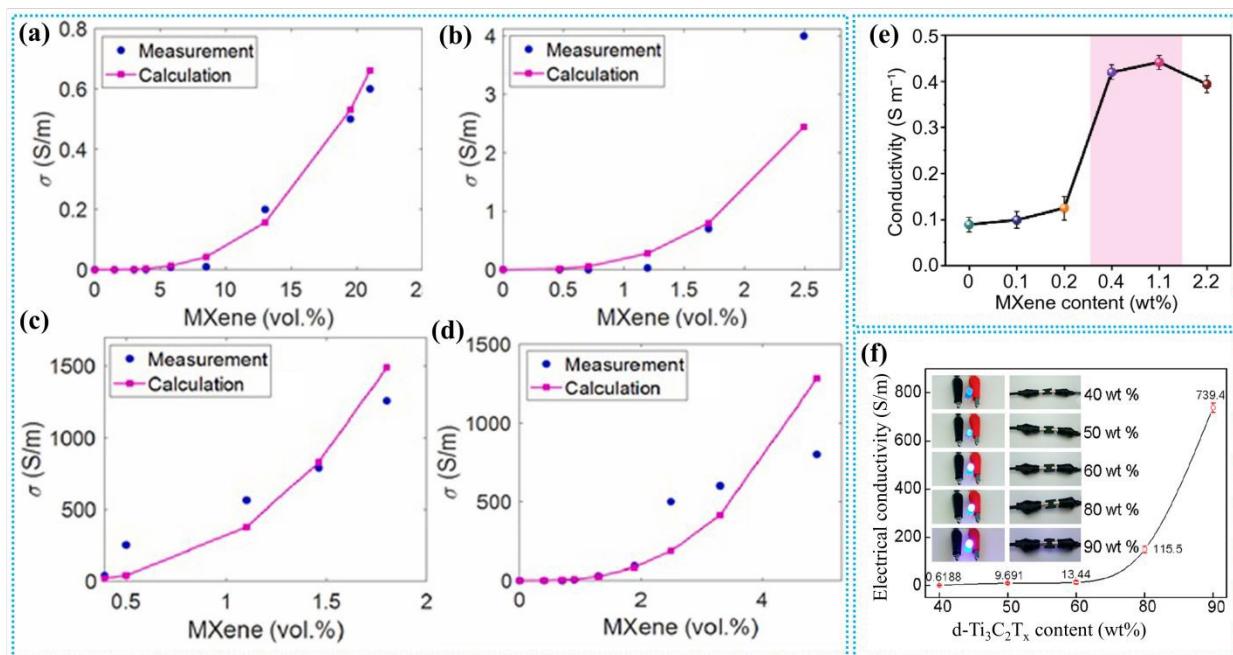
17 The role of MXene in inducing electrical conductivity in MXene-polymer nanocomposites has  
 18 been theoretically predicted for various nanocomposites like polypropylene (PP)/MXene, nitrile  
 19 butadiene rubber (NBR)/MXene, natural rubber (NR)/MXene, polystyrene (PS)/MXene, and  
 20 polyacrylamide (PAM)/MXene<sup>180</sup>. A proposed model predicts electrical conductivity, assuming



the MXene nanosheet thickness  $\sim 500$  nm. The percolation threshold ( $\varphi_p$ ), calculated using the interphase thickness aligns with experimental values. The  $\varphi_p$  is given by equation:

$$\varphi_p = \frac{(40t)^2}{(D + 20t_i)^2}$$

where  $t$  is the thickness,  $t_i$  the interphase depth, and  $D$  the MXene diameter. Uniform MXene dispersion lowers the percolation threshold, while clustering increases it. Based on theoretical predictions, the interphase thickness for NBR/MXene, PP/MXene, PS/MXene, NR/MXene, and PAM/MXene nanocomposites are 10, 10, 34, 17, and 5 nm, respectively. The proposed model yields a tunneling distance of 0.76 to 7.5 nm, which is below the 10 nm maximum threshold for tunneling conductivity. For all MXene-based nanocomposites, the theoretical calculations match with experimental values (Figure 9a-d).



**Figure 9.** Electrical properties of MXene-polymer nanocomposites. (a-d) Empirical findings and conductivity predictions for NBR/MXene, PP/MXene, PS/MXene, and NR/MXene nanocomposites, respectively. Reproduced with permission from ref.<sup>180</sup>. Copyright 2024, Elsevier Ltd. (e) Conductivity variation of MXene hydrogel with MXene content<sup>181</sup>. (f) Electrical conductivity vs. d-Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> content for d-Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/CNF composite sheets. Reproduced with permission from ref.<sup>182</sup>. Copyright 2018, American Chemical Society.

Yu et al. developed an MXene organohydrogen incorporating glycerol (Gly), featuring an MXene network for electron conduction, binary solvent channels for ion conduction, and multiple solvent-polymer-MXene interfaces for EMI applications<sup>181</sup>. The conductivity of the MXene hydrogel rises

1 sharply from 0.099 to 0.442 S m<sup>-1</sup> with increasing MXene content from 0.1 to 2.2 wt%, before  
2 slightly decreasing to 0.394 S m<sup>-1</sup>. (Figure 9e). This trend reflects the balance between enhanced  
3 electron transport and reduced ion conduction due to smaller ion channels at higher MXene  
4 concentrations.

5 MXenes, when combined with cellulose nanofibers (CNFs), form a composite paper that  
6 demonstrates significant improvements in electrical conductivity<sup>182</sup>. As the d-Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> content  
7 increases, the conductivity rises sharply, reaching 739.4 S m<sup>-1</sup> at 90 wt%. Even at 50 wt%, the  
8 conductivity is 9.691 S m<sup>-1</sup>, exceeding the 1 S m<sup>-1</sup> required for effective EMI shielding  
9 applications (Figure 9f). While the insulating nature of CNFs slightly reduces the overall  
10 conductivity compared to pure d-Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>, their one-dimensional structure aids in the alignment of  
11 MXene nanosheets, ensuring a connected and efficient conductive network. This nanocomposite  
12 exhibits a tensile strength of 135.4 MPa, a fracture strain of 16.7%, and a high folding endurance  
13 of up to 14,260 cycles.

14 MXene-based nanocomposites display both isotropic and anisotropic electrical properties,  
15 depending on their structural alignment and processing conditions. When hybridized with  
16 materials like CNTs and PVDF, these composites can exhibit anisotropic conductivity, with high  
17 in-plane conductivity and lower through-plane conductivity in films, while achieving isotropic  
18 conductivity in foams. Le et al. prepared PVDF/CNT/MXene films and introduced foam structures  
19 using CO<sub>2</sub>-assisted foaming at various saturation temperatures (T<sub>sat</sub>) and different MXene content  
20 levels. CNTs intertwine with MXenes to form a 3D conductive network, further improving  
21 electrical performance. PVDF is selected for its pyroelectric effect, high dielectric constant,  
22 mechanical stiffness, and thermal stability. The in-plane conductivity ( $\sigma_{||}$ ) and through-plane  
23 conductivity ( $\sigma_{\perp}$ ) of PVDF/CNT/MXene films initially increase with MXene content but level off  
24 due to contact resistance between fillers. At 1 wt% MXene,  $\sigma_{||}$  reaches a peak value (~17 S/m) due  
25 to optimal MXene alignment, while  $\sigma_{\perp}$  remains lower due to poor conductivity between layers.  
26 Higher MXene content (12 wt%) leads to aggregation, reducing  $\sigma_{||}$  and increasing  $\sigma_{\perp}$  slightly.  
27 Composite foams, prepared at T<sub>sat</sub> = 171 °C, show increased  $\sigma_{\perp}$  and decreased  $\sigma_{||}$  compared to  
28 films, with more random filler orientation enhancing through-plane connectivity. Larger cell sizes  
29 at higher T<sub>sat</sub> reduce filler contact, lowering both conductivities. Some of the electrical properties  
30 of MXene-polymer nanocomposites are summarized in Table 3.



1 **Table 3. Electrical properties of MXene-polymer nanocomposites**

| S. No. | Polymer        | MXene   | MXene Concentration | Electrical Conductivity (S/m) | Ref. |
|--------|----------------|---|---------------------|-------------------------------|------|
| 1      | Natural rubber | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 6.71 vol. %         | 1400                          | 167  |
| 2      | PEDOT:PSS      | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 88 wt.%             | 340.5                         | 169  |
| 3      | Epoxy          | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 15 wt.%             | 105                           | 176  |
| 4      | Epoxy          | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 4.25 wt.%           | 184                           | 165  |
| 5      | PDMS           | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 2.5 vol%            | 550                           | 183  |
| 6      | PVA            | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 90 wt.%             | 22433                         | 163  |
| 7      | PEO            | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 1 % wt.%            | $210 \times 10^{-6}$          | 184  |
| 8      | PAM            | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 6 wt.%              | $3.3 \times 10^{-2}$          | 185  |
| 9      | PVA            | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 0.14 wt.%           | $590 \times 10^{-6}$          | 186  |
| 10     | Polystyrene    | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 0.26%               | 1081                          | 187  |
| 11     | PVDF-TrFE-CFE@ | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 19.5 wt.%           | 37.4                          | 188  |

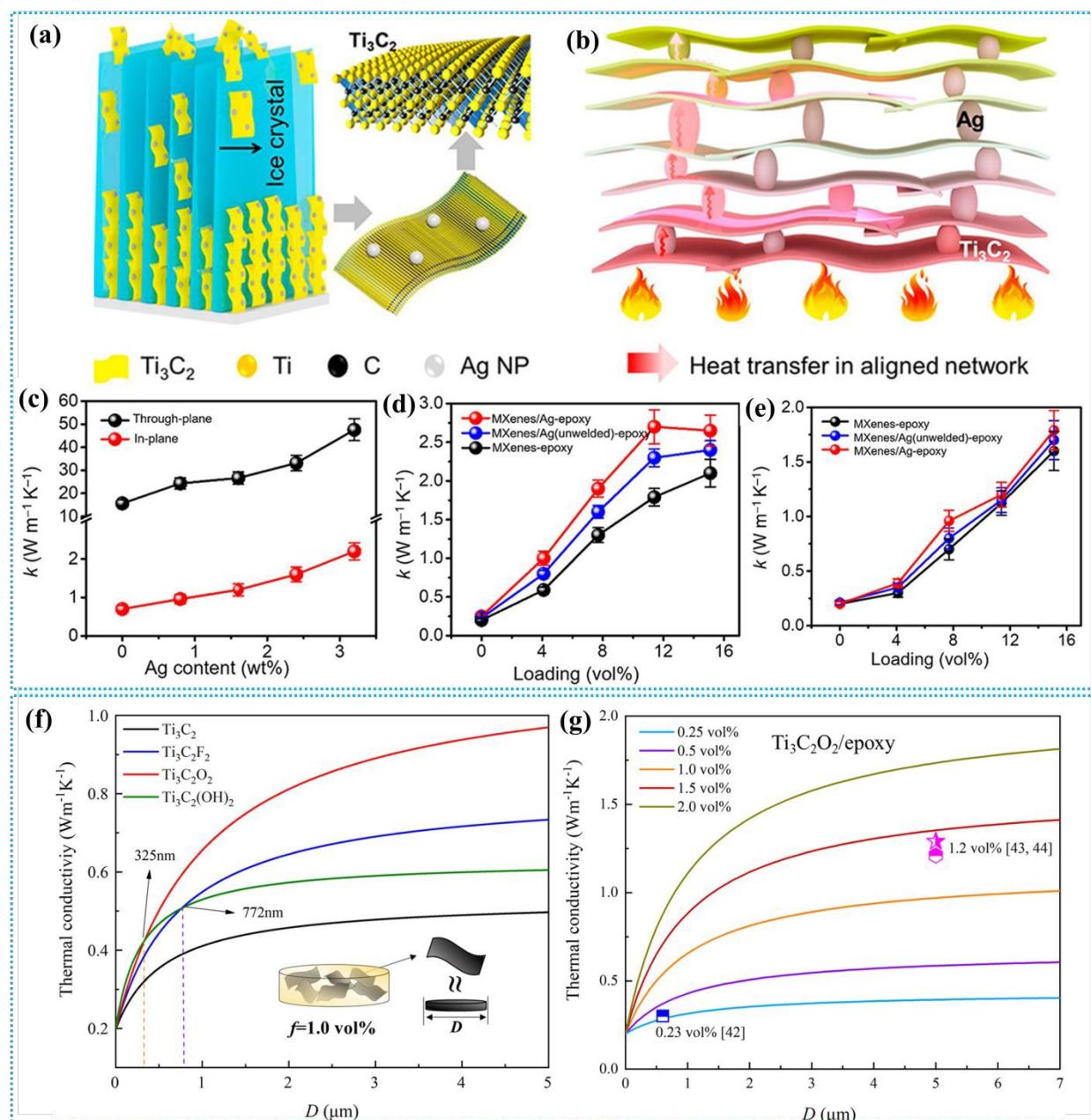
2 @poly(vinylidene fluoride-trifluoro ethylene) (PVDF-TrFE)

3 **5.3 Thermal Properties**

4 MXenes display anisotropic properties due to their structural makeup, with strong covalent bonds  
 5 within the basal plane providing high in-plane strength, while weaker interlayer forces allow easy  
 6 exfoliation<sup>189</sup>. This anisotropy results in higher thermal conductivity within the plane, making  
 7 MXenes ideal for heat dissipation in different applications<sup>190</sup>. MXenes, particularly Ti<sub>3</sub>C<sub>2</sub>, have  
 8 thermal conductivities that often surpass those of many metals, making them ideal for enhancing  
 9 heat transfer in composites. When incorporated into polymers, MXenes improve thermal  
 10 conductivity by forming interconnected networks that facilitate efficient heat conduction. The  
 11 effectiveness of these composites depends on the polymer type; those that form hydrogen bonds  
 12 with MXenes, like PVA and PVDF, enhance thermal transfer through better interfacial bonding.  
 13 The loading amount of MXenes also influences conductivity, with significant improvements  
 14 occurring when a continuous network is established at higher concentrations. First-principles  
 15 density functional calculations show that MXenes exhibit thermal conductivities greater than most  
 16 metals and low-dimensional semiconductors, making them promising additives for enhancing the  
 17 thermal conductivity of polymer composites. Earlier studies demonstrate that a Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/PVA  
 18 membrane (12.71 wt% PVA) demonstrated a thermal conductivity of 47.6 W m<sup>-1</sup>·K<sup>-1</sup>, which,



while lower than that of pristine  $\text{Ti}_3\text{C}_2$  ( $55.8 \text{ W m}^{-1}\text{K}^{-1}$ )<sup>191</sup>. Cao et al. found that the thermal conductivity of  $\text{Ti}_3\text{C}_2\text{T}_x/\text{PVDF}$  membranes exhibited minimal increase at low MXene loading (<1.0 wt%) but surged at higher levels<sup>192</sup>. This increase is attributed to the extensive surface area of  $\text{Ti}_3\text{C}_2$  flakes and the formation of hydrogen bonds with PVDF, which effectively reduce interfacial thermal resistance and enhance thermal conductivity.



**Figure 10.** Thermal properties of MXene-polymer nanocomposites. (a) Illustration of the ice-template technique for aligning MXene/Ag nanofillers. (b) Effective heat transfer in both in-plane and through-plane directions within the welded MXene/Ag aerogel skeleton due to material and

1 structural synergy. (c) Thermal conductivities of MXene films with varying Ag loadings. (d)  
2 Through-plane conductivity comparisons of MXene-epoxy, MXene/Ag (unwelded)-epoxy, and  
3 MXene/Ag-epoxy nanocomposites. (e) In-plane conductivity comparisons of MXene-epoxy,  
4 MXene/Ag (unwelded)-epoxy, and MXene/Ag-epoxy nanocomposites. Reproduced with  
5 permission from ref.<sup>193</sup>. Copyright 2020, American Chemical Society. (f) Thermal conductivity of  
6  $Ti_3C_2T_x$ /epoxy composites at 1.0 vol% filler content. (g) Thermal conductivities of  $Ti_3C_2O_2$ /epoxy  
7 composites with varying volume content and filler size. Reproduced with permission from ref.<sup>194</sup>.  
8 Copyright 2022, Elsevier Ltd.

9 To improve the thermal conductivity of the MXene/epoxy nanocomposites Ji et al. designed 3D  
10 MXene/Ag aerogels using the ice templating method (Figure 10a) as heat transfer skeletons for  
11 epoxy nanocomposites by in situ decorating Ag nanoparticles on exfoliated MXene nanosheets to  
12 improve contact<sup>193</sup> (Figure 10b). The vertically aligned MXenes, with a high through-plane  
13 thermal conductivity of  $472\text{ W m}^{-1}\text{ K}^{-1}$ , form a thermally conductive network when combined  
14 with Ag, which has a thermal conductivity of  $430\text{ W m}^{-1}\text{ K}^{-1}$  and low soldering temperature. The  
15 resulting MXene/Ag/epoxy nanocomposite exhibits a through-plane thermal conductivity of  $2.65\text{ W m}^{-1}\text{ K}^{-1}$ , a 26.2% increase compared to the MXene-epoxy nanocomposite, along with improved  
16 mechanical and thermal expansion properties. The films demonstrate distinct thermal conductive  
17 behaviors in the in-plane and through-plane directions, with in-plane thermal conductivity rising  
18 to  $47.57\text{ W m}^{-1}\text{ K}^{-1}$  at 3.2 wt% Ag nanoparticles loading compared to  $15.64\text{ W m}^{-1}\text{ K}^{-1}$  for pristine  
19 MXene films. In the through-plane direction, the thermal conductivity increases from 0.7 to  $2.2\text{ W m}^{-1}\text{ K}^{-1}$  (Figure 10c), enhancing efficient heat dissipation in practical applications; however, Ag  
20 nanoparticles loading beyond 3.2 wt% leads to film fragility. The thermal conductivities of  
21 MXene/Ag/epoxy nanocomposites, measured via the laser flash technique, exhibited  
22 enhancements in both in-plane (Figure 10d) and through-plane (Figure 10e) directions upon  
23 incorporating MXene/Ag fillers. The through-plane thermal conductivity reaches  $2.65\text{ W m}^{-1}\text{ K}^{-1}$   
24 at 15.1 vol% filler loading, representing a >1200% increase compared to pure epoxy resin. This  
25 suggests that Ag nanoparticles improve thermal conductivity by promoting effective heat transfer  
26 channels within the nanocomposite. The observed anisotropic thermal behavior is attributed to the  
27 two-dimensional structure of MXenes, which results in distinct heat transfer mechanisms along  
28 the horizontal and vertical orientations of the film.

31 Terminal groups on MXenes can impact thermal conductivity by reducing phonon scattering and  
32 enhancing interfacial interactions with epoxy matrices<sup>194, 195</sup>. Wang et al. used molecular dynamics  
33 and effective medium theory to analyze four MXenes- $Ti_3C_2$ ,  $Ti_3C_2F_2$ ,  $Ti_3C_2O_2$ , and  $Ti_3C_2(OH)_2$ -



and their epoxy composites<sup>194</sup>. The study found that  $\text{Ti}_3\text{C}_2\text{O}_2$  achieves the highest thermal conductivity of  $140.25 \text{ W m}^{-1} \text{ K}^{-1}$ , while  $\text{Ti}_3\text{C}_2(\text{OH})_2$  exhibits the lowest interfacial thermal resistance (ITR), improving composite conductivity at optimal flake sizes (Figure 10f). The study assumes MXene flakes as disk shapes with a diameter and thickness of 0.98 nm. It was proposed that the effective thermal conductivities of the nanocomposites initially increase sharply with the lateral size of fillers, eventually leveling off after reaching a critical size. Among the composites,  $\text{Ti}_3\text{C}_2\text{O}_2/\text{epoxy}$  demonstrates the highest thermal conductivity, while  $\text{Ti}_3\text{C}_2/\text{epoxy}$  exhibits the lowest due to its intrinsic thermal conductivity and high ITR. The results indicate two intersections between  $\text{Ti}_3\text{C}_2(\text{OH})_2/\text{epoxy}$  and the -O and -F terminated MXenes, suggesting that below critical sizes (325 nm for -O and 772 nm for -F), interfacial thermal conductance plays a more significant role in enhancing thermal performance. Additionally, in the  $\text{Ti}_3\text{C}_2\text{O}_2/\text{epoxy}$  system, filler volume content below 2 vol% is optimal to avoid agglomeration, with thermal conductivity increasing linearly before reaching a plateau as the MXene size increases (Figure 10g). Some of the thermal properties of MXene-polymer nanocomposites are summarized in Table 4.

**Table 4. Thermal properties of MXene-polymer nanocomposites**

| S. No. | Polymer                          | MXene                             | MXene Concentration | Thermal Conductivity (W/mK) | Improvement percentage (%) | Ref. |
|--------|----------------------------------|-----------------------------------|---------------------|-----------------------------|----------------------------|------|
| 1      | PVA                              | $\text{Ti}_3\text{C}_2\text{T}_x$ | 2 wt.%              | -                           | 18.7                       | 170  |
| 2      | Thermoplastic polyurethane (TPU) | $\text{Ti}_3\text{C}_2\text{T}_x$ | 1 wt.%              | -                           | 8.4                        | 172  |
| 3      | PVC                              | $\text{Ti}_3\text{C}_2\text{T}_x$ | 15 wt.%             | 3.45                        | ~1050                      | 173  |
| 4      | PVA                              | $\text{Ti}_3\text{C}_2\text{T}_x$ | 2 wt.%              | -                           | 8.2                        | 174  |
| 5      | Epoxy                            | $\text{Ti}_3\text{CN}$            | 5 wt.%              | -                           | 2.7                        | 175  |
| 6      | Epoxy resin                      | $\text{Ti}_3\text{C}_2\text{T}_x$ | 1.0 wt.%            | -                           | -0.55                      | 168  |
| 7      | Polypropylene                    | $\text{Ti}_3\text{C}_2\text{T}_x$ | 2.0 wt.%            | -                           | 11.8                       | 177  |
| 8      | PDMS                             | $\text{Ti}_3\text{C}_2\text{T}_x$ | 2.5 vol%            | 0.694                       | 220                        | 183  |
| 9      | PVDF                             | $\text{Ti}_3\text{C}_2\text{T}_x$ | 5 wt.%              | 0.363                       | 100                        | 196  |
| 10     | PVA                              | $\text{Ti}_3\text{C}_2\text{T}_x$ | -                   | 47.6                        | -                          | 197  |
| 11     | Epoxy                            | $\text{Ti}_3\text{C}_2\text{T}_x$ | 15 wt.%             | 7.60                        | ~100                       | 198  |
| 12     | Epoxy                            | $\text{Ti}_3\text{C}_2\text{T}_x$ | 1 wt.%              | 0.587                       | 141.3                      | 199  |

## 6. MXene-polymer nanocomposites- synthesis strategies



1 MXenes can be integrated with a wide range of polymers, facilitating the tailoring of  
2 nanocomposite materials for specific applications. The interaction force between the MXene  
3 matrix and polymers in nanocomposite synthesis primarily involves hydrogen bonding, van der  
4 Waals interactions, electrostatic interactions, and  $\pi$ - $\pi$  stacking, depending on the functional groups  
5 present on both MXene surfaces and the polymer chains<sup>94</sup>. The MXene surface terminations (e.g.,  
6 –O, –OH, –F,) can form hydrogen bonds with polymers containing polar groups like –OH, –  
7 COOH, –NH<sub>2</sub>, etc. Additionally, electrostatic interactions may occur when charged polymers are  
8 used, especially in systems where MXenes have surface charges<sup>92</sup>. Van der Waals forces contribute  
9 to non-covalent binding, while polymers with aromatic groups can engage in  $\pi$ - $\pi$  interactions with  
10 MXene layers. These interactions are key to enhancing compatibility, mechanical strength, and  
11 functional properties in MXene-polymer nanocomposites. MXene-polymer composites can be  
12 fabricated using different processing techniques, such as solution casting<sup>68, 77</sup>, melt blending<sup>200, 201</sup>,  
13 or electrospinning<sup>80</sup>, etc., allowing for the production of complex shapes, thin films, coatings, or  
14 fibers. This versatility in processing enables the integration of MXenes into a wide range of devices  
15 and structures<sup>202, 203, 204, 205</sup>.

### 16 **6.1 Surface grafting/modification of MXenes**

17 Due to the abundant functional groups at the surface of MXenes, it becomes easier to functionalize  
18 these with different organic molecules. First-principles calculations revealed that unmodified  
19 Ti<sub>3</sub>C<sub>2</sub> MXene can cleave and decompose monomers effectively. In contrast, surface-functionalized  
20 Ti<sub>3</sub>C<sub>2</sub>F<sub>2</sub>, Ti<sub>3</sub>C<sub>2</sub>FO, and Ti<sub>3</sub>C<sub>2</sub>O<sub>2</sub> bind weakly with monomers due to van der Waals forces, while  
21 Ti<sub>3</sub>C<sub>2</sub>(OH)<sub>2</sub> shows a stronger binding affinity<sup>206</sup>. In the surface modification process, MXene  
22 sheets are functionalized or chemically modified to introduce specific groups or moieties on their  
23 surfaces. These modified MXene sheets are then mixed or dispersed within a polymer solution or  
24 melt. During polymerization or crosslinking, the functionalized MXene sheets become covalently  
25 bonded or physically intertwined with the polymer chains, leading to the formation of  
26 nanocomposite material<sup>207, 208</sup>. A protein-inspired supramolecular elastomer was developed for  
27 intelligent sensing applications, utilizing self-healable Ti<sub>3</sub>C<sub>2</sub> MXene blended with rubber (serine-  
28 grafted epoxidized natural rubber) (S-ENR) latex<sup>209</sup>. The study created a self-healing elastomer  
29 inspired by proteins for smart sensing. MXene nanosheets were esterified with serine using EDC  
30 and DMAP at 100°C for 3 hours to produce S-MXene (Figure 11a). Serine-modified epoxidized  
31 natural rubber (ENR) latex was synthesized by reacting serine with ENR latex at 100°C for 3

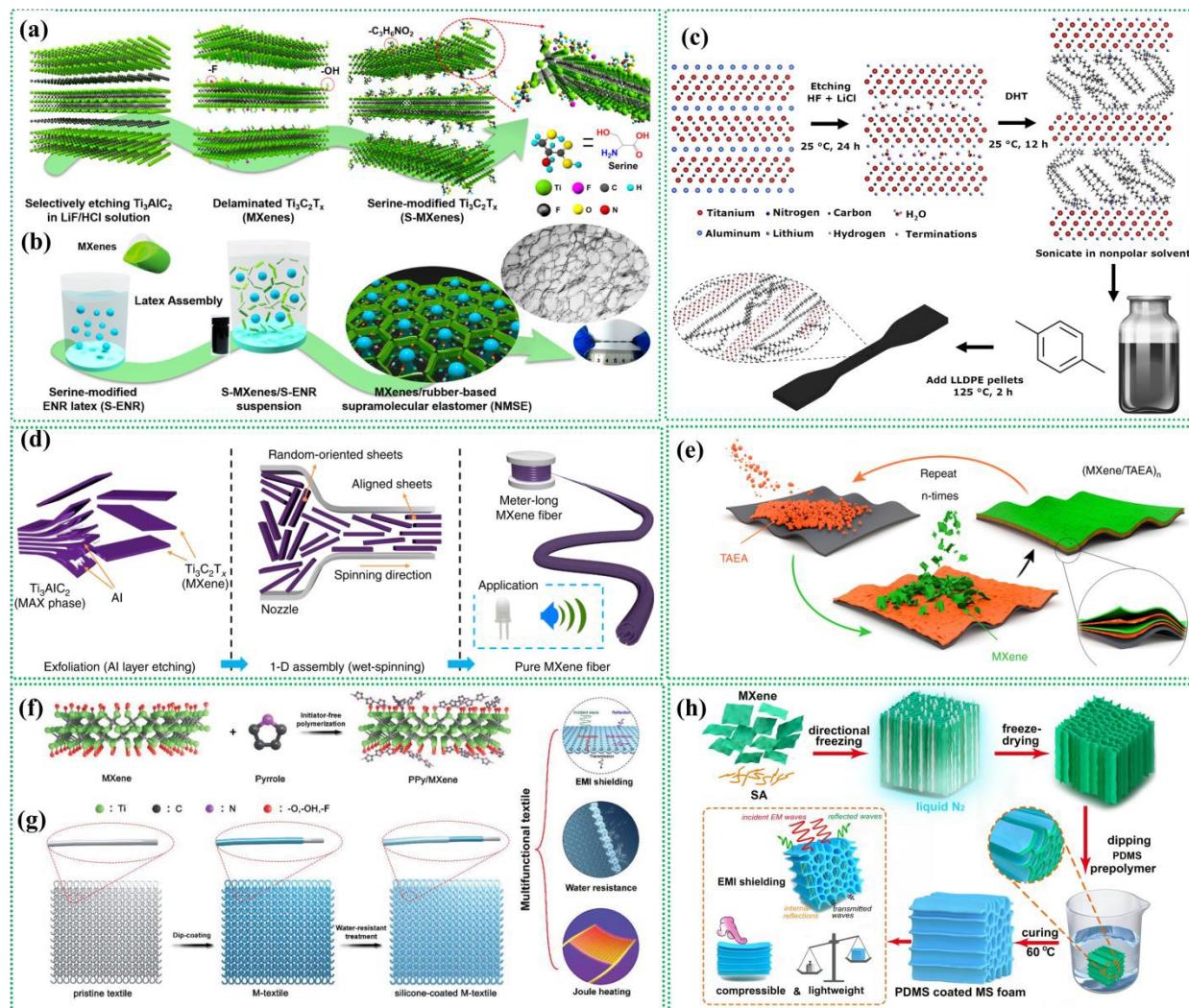


hours. S-MXenes/S-ENR nanocomposites were prepared by combining S-MXene with S-ENR latex, stirring, sonicating, and drying to form a 3D network film (Figure 11b). Besides this, another surface modification technique involving the covalent attachment of polyethylene glycol carboxylic acid (PEG6-COOH), onto MXenes through esterification chemistry was introduced. The surface modification of  $Ti_3C_2T_x$  using PEG6-COOH with high ligand loading significantly improves the dispersibility of MXene flakes in a wide range of non-polar organic solvents (e.g., 2.88 mg/mL in chloroform) without inducing oxidation or altering the structural ordering of  $Ti_3C_2T_x$  two-dimensional layers<sup>208</sup>. Besides these, there are other reports on the MXenes surface modifications for MXene-polymer hybridization<sup>208, 210</sup>.

## 6.2 Solution blending

In this method, MXenes and polymers are dispersed in a compatible solvent, and mixed via stirring, ultrasonication, or high-shear mixing. Then the solvent is removed by evaporation, vacuum drying, or freeze-drying to form a solid MXene-polymer composite. Carey et.al conducted a study where they prepared a dispersion of alkylated 2D MXene in nonpolar solvents using the blending method<sup>201</sup>. The study investigated the pseudocapacitive behavior of the resulting nanocomposite material. In this process, after the MXene etching, the  $Li^+$  ions present inside the multilayers are ion-exchanged with di(hydrogenated tallow)benzyl methyl ammonium chloride (DHT) (Figure 11c). The resulting multilayers can be easily dispersed in nonpolar solvents. These can be easily processed with linear low-density polyethylene nanocomposite (LLDPE) for many applications. The good part of this hybrid assembly is that these remain dispersed for more than 10 days without sedimenting even in nonpolar solvents. Jiao et.al conducted a study to prepare photothermal healable, stretchable, and conductive  $Ti_3C_2T_x$  MXene composite films using the vacuum filtration method, to achieve efficient EMI shielding<sup>211</sup>. To determine the optimal ratio between waterborne polyurethane (WPU) and natural rubber latex (NR latex), a series of composite films were prepared with varying WPU: NR mass ratios. These composite films were respectively denoted as WNM as these contain WPU, NR, and MXene. The next step involved obtaining WPU/NR composite emulsions by mixing specific proportions of WPU and NR latex emulsions in an ice bath. Subsequently, a  $Ti_3C_2T_x$  suspension was gradually introduced into the WPU/NR composite emulsions. This step allowed the incorporation of  $Ti_3C_2T_x$  at various volume fractions.





**Figure 11.** MXene-polymer nanocomposites synthesis. (a) The surface modification of MXene nanosheets is achieved through an esterification reaction with serine. (b) MXene network in NMSE is constructed using the latex assembly method. Reproduced with permission from ref.<sup>209</sup>. Copyright 2020, American Chemical Society. (c) MXene-polymer blending. MXene multilayers are then treated with DHT to enhance their functionality. The functionalized MXene nanosheets are dispersed in a nonpolar solvent and subsequently utilized in the solution processing of LLDPE<sup>201</sup>. (d) Electrospinning technique. MXene material is concentrated in an aqueous solution and then assembled into a fiber. This fiber was aligned in the axial direction using a wet-spinning process<sup>212</sup>. (e) The process of LBL self-assembly of  $(MXene/TAEA)_n$  multilayer films on planar substrates is depicted schematically<sup>213</sup>. (f) In-situ polymerization MXene-polymer hybrids. Schematic illustration of the modification process of MXene with in situ polymerized PPy. (g) Fabrication of PPy/MXene-decorated PET textile, along with the subsequent process of creating the multifunctional silicone-coated M-textile. Reproduced with permission from ref.<sup>82</sup>. Copyright 2018, Wiley. (h) The schematic shows the process of making an MXene/SA hybrid aerogel and its subsequent PDMS-coated MXene/SA foam. Reproduced with permission from ref.<sup>214</sup>. Copyright 2024, Elsevier Ltd.

1 The WNM films were obtained through vacuum filtration, followed by natural drying. Recently,  
2 Pan et al. have reported a wearable and flexible MXene and PEDOT: PSS conducting polymer  
3 nanocomposite for continuous noninvasive monitoring of sweat glucose<sup>215</sup>. The addition of 0.1 %  
4 mass fraction of MXene has significantly improved the conductivity of the composite. In this  
5 study, ethylene glycol has been utilized to increase the cross-linking and film-forming properties  
6 of nanocomposite. The nanocomposite hydrogel sensor showed a sensitivity of  $21.7 \mu\text{A}\cdot\text{mM}^{-1}$   
7  $\text{cm}^{-2}$  within the concentration range of 1–94  $\mu\text{M}$  and a sensitivity of  $8.3 \mu\text{A}\cdot\text{mM}^{-1}\text{cm}^{-2}$  within the  
8 range of 94–1294  $\mu\text{M}$ . Importantly, this glucose biosensor demonstrated outstanding  
9 electrochemical performance in sweat, which was highly correlated with the corresponding  
10 findings of the glucometer.

### 11 **6.3 Electrospinning method**

12 The electrospinning technique can prepare polymer fibers with diameters in the nanoscale range.  
13 MXene-polymer nanocomposites can be effectively synthesized using electrospinning  
14 techniques<sup>80, 216</sup>. MXene fibers can also be synthesized using the wet-spinning technique. Eom et  
15 al. devised a technique for producing pure MXene fibers without additional binders<sup>212</sup>. This  
16 method involves a large-scale wet-spinning assembly, where MXene sheets are dispersed in water  
17 at high concentrations, preventing aggregation or phase separation issues (Figure 11d). The  
18 coagulation process plays a pivotal role in the fabrication of these fibers. By introducing  
19 ammonium ions during coagulation, the researchers have assembled MXene sheets into highly  
20 flexible, meter-long fibers. These fibers exhibit an exceptionally high level of electrical  
21 conductivity, making them promising candidates for various applications in advanced materials.  
22 Besides, MXenes can be incorporated into polymer solutions used for electrospinning to produce  
23 MXene-polymer composite nanofibers. Recently, a study was conducted on an electrospun  
24 flexible triboelectric nanogenerator that utilized metallic MXene nanosheets and poly(vinyl  
25 alcohol) (PVA)<sup>217</sup>. To prepare the PVA-MXene solution, a 10% (w/v) PVA solution, 1.0 g of PVA  
26 was mixed with 10 mL of distilled water at 90 °C while stirring for ~1 h. Subsequently, MXene  
27 was added to the PVA aqueous solution and stirred thoroughly to achieve a homogeneous  
28 PVA/MXene mixture. Electrospinning was performed using a 5 mL syringe and needle with a 0.68  
29 mm inner diameter at an applied voltage of 18 kV. The combination of MXene nanosheets and  
30 PVA in the composite material imparts outstanding electrical properties, enhancing its  
31 electronegativity and conductivity. For the positive friction layer, silk fibroin (SF) was selected as



1 the material for electrospinning nanofiber film due to its biocompatibility, biodegradability, and  
2 significant triboelectric properties.

### 3 **6.4 Layer-by-layer (LBL) assembly**

4 This method involves the sequential deposition of alternating layers of  $Ti_3C_2T_x$  MXenes and  
5 polymers onto a substrate. The MXene and polymer layers are formed through techniques such as  
6 dip coating, spin coating, spray deposition, etc. The coating process can be repeated to achieve the  
7 desired thickness and control the MXene-to-polymer ratio in the composite. A method for the  
8 vacuum-assisted LBL self-assembly of pillared two-dimensional multilayers comprising MXene  
9 and a small molecule called tris(2-aminoethyl) amine (TAEA) was developed<sup>213</sup>. In this process,  
10 (*MXene/TAEA*)*n* multilayers were prepared, where *n* represents the number of bilayers formed in  
11 the self-assembled structure. In this method,  $Ti_3C_2T_x$  MXene and TAEA solutions with a  
12 concentration of  $1\text{ g L}^{-1}$  were used. Porous substrates were placed on a cellulose membrane fixed  
13 in an adjustable-flow vacuum system. Using airbrushes, atomized solutions were sprayed onto the  
14 substrates. The cycle of spraying TAEA, rinsing with water, and then spraying MXene was  
15 repeated to create (*MXene/TAEA*)*n* films of the desired thickness (Figure 11e). For larger surfaces  
16 of 3D CNF aerogel and melamine foam, a rapid-LBL assembly method was used. MXene and  
17 TAEA solutions were poured on top of the aerogel or foam and forced through by applying vacuum  
18 pressure. (*MXene/TAEA*)*n* multilayer films can be prepared through LBL self-assembly onto  
19 fibers and foams. Another study was conducted titled LBL assembly of polyaniline nanofibers  
20 (PNF) and  $Ti_3C_2T_x$  MXene electrodes for electrochemical energy storage<sup>218</sup>. In this research, the  
21 LBL assembly technique was used to create thin-film electrodes by stacking PNF and  $Ti_3C_2T_x$   
22 MXene materials. The resulting electrodes were intended for applications in electrochemical  
23 energy storage, aiming to enhance the performance of energy storage devices such as batteries or  
24 supercapacitors.

### 25 **6.5 In-situ polymerization**

26 In this method, the monomers of the polymer are introduced into a solution containing MXene,  
27 and polymerization occurs *in situ*, meaning within the same environment as the MXene particles<sup>81,</sup>  
28 <sup>82, 214</sup>. This leads to the formation of a homogeneous mixture of MXene and polymer, creating a  
29 nanocomposite material with MXene uniformly dispersed throughout the polymer matrix<sup>219</sup>. The  
30 choice of polymer depends upon the end requirement. If a conducting polymer is chosen it will  
31 result in a nanocomposite which may have applications as active electronic material whereas, an



insulating polymer will result in a final product with limited or reduced conductivity. In a study reported by Wang et al., the fabrication of MXene-decorated multifunctional and water-resistant textiles with remarkable electromagnetic interference (EMI) shielding and Joule heating performances were investigated. To achieve this, PPy modified MXene sheets using in-situ polymerization (Figure 11f) were utilized, which were deposited onto poly(ethylene terephthalate) textiles<sup>82</sup>. Subsequently, a silicone coating was applied to the textiles to enhance their conductivity and hydrophobicity. Highly conductive and water-resistant textiles exhibited high EMI shielding efficiency and excellent Joule heating performance (Figure 11g). In another study, Wu and co-workers developed compressible, durable, and conductive PDMS-coated MXene/sodium alginate (SA) foams (MS) for high-performance electromagnetic interference (EMI) shielding. The researchers used MXene and SA to fabricate the foam and then coated the foam with PDMS to enhance its properties for EMI shielding<sup>214</sup>. Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>/SA hybrid aerogels were fabricated as follows: Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> suspension (20 mg mL<sup>-1</sup>) was added to different amounts of SA (0, 4, 12, 28, and 48 mg) with stirring at 500 rpm for 5 h to achieve homogeneous and high viscosity suspensions. The resulting suspensions were poured into Teflon molds and rapidly frozen on a copper cylinder immersed in liquid nitrogen. Subsequently, the directionally frozen samples were freeze-dried at -60 °C under 10 Pa for 48 h to yield unidirectional aerogels. These MS porous architectures were coated with PDMS by vacuum-assisted impregnation method. To create the PDMS-coated MS foam, a mixture of 10 g PDMS prepolymer, 1 g curing agent, and 30 mL n-hexane was thoroughly mixed in a beaker for 30 min. The resulting mixture was cured at 60 °C for 12 h, resulting in the formation of a thin PDMS layer on the MXene nanosheets of the MS aerogel, creating the PDMS-coated MS foam (Figure 11h). The resulting PDMS-coated MXene/SA foam exhibited excellent compressibility, durability, and electrical conductivity, making it a promising candidate for effective EMI shielding applications. Besides these, Table 5 summarizes different polymers utilized in MXene-polymers nanocomposite synthesis, along with their respective applications.

**Table 5.** MXene-polymer nanocomposites and their applications.

| S. No. | MXene   | Polymer used | Synthesis technique    | MXene concentration | Application of nanocomposite | Reference      |
|--------|---|--------------|------------------------|---------------------|------------------------------|----------------|
| 1      | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PEDOT:PSS    | Electrogelation method | 0 to 60wt%          | Sensing                      | <sup>220</sup> |
| 2      | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PEDOT:PSS    | Ice templating method  | 0, 1, and 3 wt %    | Electrical stimulation       | <sup>221</sup> |
| 3      | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PEDOT:PSS    | Mixing/blending        | 10-90 wt.%          | EMI shielding                | <sup>222</sup> |



|    |   |               |                        |                                     |                                   |     |
|----|---|---------------|------------------------|-------------------------------------|-----------------------------------|-----|
| 4  | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PEDOT:PSS     | LBL assembly           | -                                   | Energy storage/capacitive sensors | 88  |
| 5  | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PEDOT:PSS     | LBL assembly (spray)   | 29- 76.6 wt%                        | Multifunctional                   | 223 |
| 6  | V <sub>2</sub> CT <sub>x</sub>                | PEDOT:PSS     | Mixing/blending        | -                                   | Solar cells                       | 224 |
| 7  | Nb <sub>2</sub> CT <sub>x</sub>               | PEDOT:PSS     | Solution mixing        | MXene:PEDOT:PSS (1:5, 1:7, and 1:9) | Solar cells                       | 225 |
| 8  | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PDMS          | Dip-coating and curing | 1, 3, and 5 wt.%                    | EMI shielding skins               | 226 |
| 9  | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PDMS          | Mixing/curing          | 20-50%                              | Pressure sensor                   | 227 |
| 10 | V <sub>2</sub> CT <sub>x</sub>                | PDMS          | Coating                | -                                   | EDL transistor                    | 228 |
| 11 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PU#           | Mixing                 | 1:1                                 | EMI shielding                     | 229 |
| 12 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PU#           | LBL assembly           | -                                   | EMI shielding and Joule Heating   | 230 |
| 13 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Epoxy         | Coating                | 0-2wt.%                             | Anti-corrosion                    | 231 |
| 14 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Polypyrrole   | In situ polymerization | MXene:PPy (9:1, 8:2 and 7:3)        | Supercapacitors                   | 232 |
| 15 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Doxorubicin   | Surface modification   | 1:2                                 | Tumor targeting                   | 233 |
| 16 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Chitosan      | Electrospinning        | 0- 0.75 wt.%                        | Antibacterial                     | 234 |
| 17 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Silane        | Surface modification   | 1:1                                 | Water purification                | 235 |
| 18 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PANI/PU       | Electrospinning        | 0- 10%                              | Zn-ion batteries                  | 236 |
| 19 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Polypyrrole   | Polymerization         | 1:1 and 2:1                         | Pseudocapacitive electrodes       | 81  |
| 20 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PEG           | 3D printing            | -                                   | Tissue engineering                | 237 |
| 21 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PVA           | Blending               | 40-90%                              | Flexible electronics              | 16  |
| 22 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | PVA           | Solvent exchange       | 2.50%                               | Strain sensors                    | 238 |
| 23 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | SA            | Ultrasonic mixing      | 5-30 mg mL-                         | Flexible electronic sen           | 239 |
| 24 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | Polypropylene | Hot-pressing           | 25%, 56%, and 70%                   | Flame-retarding/ EMI shielding    | 240 |
| 25 | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | TAEA*         | LBL self-assembly      | -                                   | Supercapacitors                   | 213 |

1 \* Tris(2-aminoethyl) amine (TAEA), #polyurethane (PU)

2 Combining MXenes with a wide variety of polymers makes it possible to enhance and tailor the  
 3 properties of MXenes and these can alter the properties of the resulting composite material as  
 4 desired<sup>241, 242, 243</sup>.

## 5 7. Applications of MXene-polymer nanocomposites



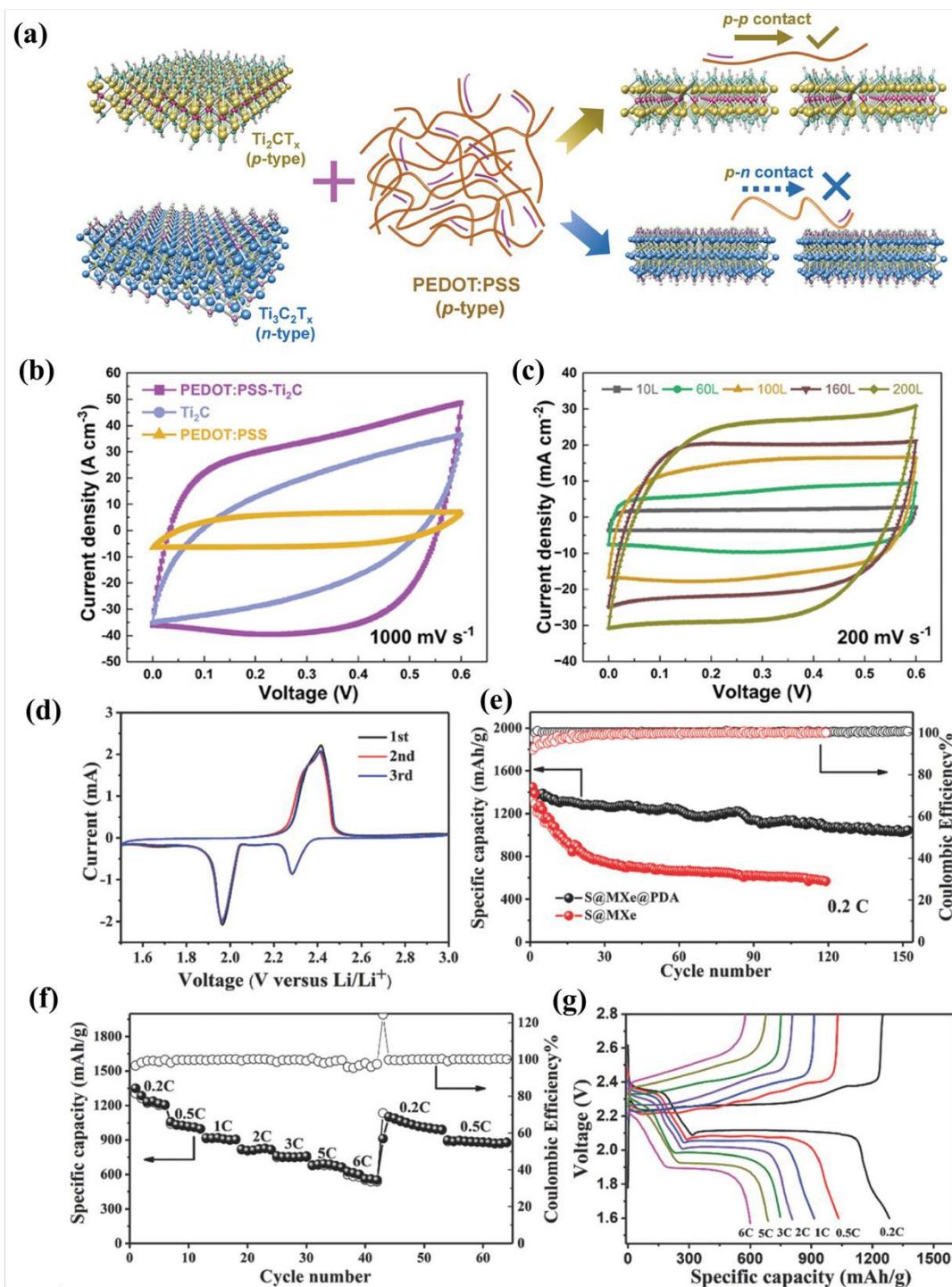
1 The addition of polymers to MXenes can significantly improve their performance and expand their  
2 applications in various fields. By incorporating polymers with good mechanical strength and  
3 flexibility, the resulting MXene-polymer hybrids exhibit enhanced mechanical properties, making  
4 them suitable for applications requiring flexibility, stretchability, and impact resistance<sup>54, 244, 245</sup>.  
5 This includes flexible electronics, wearable devices, and flexible coatings<sup>60, 83, 202, 246</sup>. Polymers  
6 can enhance the electrochemical performance of MXenes in energy storage devices. The  
7 combination of MXenes' high electrical conductivity with polymers' ion transport properties can  
8 enhance the charge storage capacity of these devices<sup>247, 248</sup>. Polymers enhance MXene dispersion,  
9 prevent restacking, and improve synergy, boosting overall material properties<sup>249</sup>.

### 10 **7.1 MXene-polymers for energy storage applications**

11 MXene-polymer composites offer several advantages in energy storage devices. Polymers can  
12 provide mechanical stability to the electrode materials. This improved mechanical stability leads  
13 to enhanced cycling performance and a longer lifespan of energy storage devices<sup>250</sup>. Due to van  
14 der Waals forces, MXenes layers tend to restack and agglomerate, resulting in reduced accessible  
15 surface area and hindered ion diffusion due to lack of active sites<sup>91, 251</sup>. Polymers in MXene-  
16 polymer composites help to disperse and stabilize MXene layers, preventing restacking and  
17 preserving the high surface area of MXenes<sup>16</sup>. Polymers can facilitate ion diffusion within the  
18 electrode materials<sup>252</sup>. Polymers can enhance the compatibility of MXene electrodes with different  
19 electrolyte systems. Certain polymers can act as ion-conductive additives or binders that promote  
20 ion transport and enhance the stability of electrolyte-electrode interfaces. The performance of the  
21 electrodes, which were fabricated using PEDOT (poly(3,4-ethylene dioxythiophene)) deposited  
22 Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> sheets, exhibited an improvement compared to the electrodes made with pristine  
23 Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub><sup>253</sup>.

24 Polyaniline@MXene-based positive electrodes have been investigated for asymmetric  
25 supercapacitor applications<sup>250</sup>. The electrode is prepared by casting a homogenous polyaniline  
26 layer onto a 3D porous Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene. This enabled the stable operation of MXene at positive  
27 potential due to the increased work function after combining with polyaniline. The resulting  
28 flexible polyaniline@MXene positive electrode offers a high volumetric capacitance of 1632 F  
29 cm<sup>-3</sup> at 5000 mV s<sup>-1</sup>. In another study, pseudocapacitive electrodes were developed by performing  
30 oxidant-free polymerization of PPy between the layers of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene<sup>81</sup>. Hybrid electrodes of  
31 Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> and PPy achieved up to 416 F g<sup>-1</sup> capacitance in 1 M H<sub>2</sub>SO<sub>4</sub>.





**Figure 12.** (a) Schematic of interactions between PEDOT:PSS and MXenes ( $\text{Ti}_2\text{C}$  and  $\text{Ti}_3\text{C}_2$ ). (b) CV curves of 10L MSCs with  $\text{Ti}_2\text{C}$ , PEDOT:PSS, and PEDOT:PSS- $\text{Ti}_2\text{C}$  electrodes. (c) CV curves of PEDOT:PSS- $\text{Ti}_2\text{C}$  MSCs at  $200 \text{ mV s}^{-1}$  with different layer numbers<sup>254</sup>. (d) CV curves of S@MXene@PDA at  $0.2 \text{ mV s}^{-1}$  (first three cycles). (e) Cycling performance of S@MXene@PDA vs. S@MXene at  $0.2 \text{ C}$ . (f, g) Rate performance and voltage profiles at  $0.2\text{--}6 \text{ C}$ . Reproduced with permission from ref.<sup>255</sup>. Copyright 2018, Wiley.

1 MXene/PPy (2:1 and 1:1 ratios) nanocomposites, prepared by mixing delaminated  $Ti_3C_2T_x$  and  
2 PPy, were utilized for supercapacitor applications. Cyclic voltammetry (CV) curves of the hybrid  
3 samples revealed a strong pseudocapacitive behavior. The supercapacitors based on a 2:1 ratio  
4 nanocomposite demonstrated higher capacitance than those of pristine MXene and the 1:1 ratio  
5 due to optimized composition. These supercapacitors outperformed PVA- $Ti_3C_2T_x$  electrodes,  
6 achieving ~99% Coulombic efficiency and 92% capacitance retention over 25,000 cycles. Nyquist  
7 plots confirmed good ionic conductivity, with slightly higher diffusion resistance in PPy-  
8 containing films, attributed to robust bonding, effective ion/electron transport, and protective role  
9 of MXene.

10 Besides  $Ti_3C_2T_x$  MXene  $Ti_2C$  MXene has also demonstrated excellent energy storage capabilities.  
11 Xue et al. developed ultrafast, metal-free, on-paper micro-supercapacitors (MSCs) using a  
12 composite of conductive PEDOT: PSS and capacitive  $Ti_2C$  MXene<sup>254</sup>. They developed a more  
13 effective direct ink writing (DIW) by combining PEDOT: PSS with  $Ti_2CT_x$ , leveraging its higher  
14 specific capacitance and compatibility with PEDOT: PSS's hole transport paths (Figure 12a).  
15 Unlike  $Ti_3C_2T_x$ , this blend avoids conductivity degradation, enabling improved conductivity,  
16 reduced restacking, and high-rate electrochemical performance even with thick electrodes. At 1000  
17 mV s<sup>-1</sup> scan rate, PEDOT: PSS- $Ti_2C$  MSCs (10 layers, ≈5 μm thick) achieved a volumetric  
18 capacitance of ≈30.6 F cm<sup>-3</sup>, which is nearly double that of pure  $Ti_2C$  MSCs and 6 times higher  
19 than PEDOT: PSS MSCs, confirming their synergistic interaction. CV curves maintained excellent  
20 rectangularity, and capacitance increased linearly with layer count at lower scan rates (Figure 12b-  
21 c). These MSCs retained >96% of their capacitance after 10,000 cycles at a high scan rate of 1000  
22 mV s<sup>-1</sup>. They also exhibited an extended voltage window of up to 6 V and maintained outstanding  
23 performance even at ultrafast scan rates of 10 V s<sup>-1</sup>. This work highlights the potential of  $Ti_2C$   
24 when integrated with polymers for eco-friendly, high-performance power sources for paper-based,  
25 portable, and wearable electronics. Additionally, flexible solid-state micro-supercapacitors can be  
26 fabricated by electrochemically polymerizing MXene-facilitated PEDOT composite films, and  
27 these composite films can be utilized along with  $MnO_2$  to create pseudocapacitive asymmetric  
28 micro-supercapacitors<sup>256</sup>.

29 MXene-polymer nanocomposites also offer advantages in batteries, as demonstrated by Yiao et al.  
30 in Li-S batteries with MXene-polydopamine (S@Mxe@PDA) cathodes<sup>255</sup>. The dual polysulfide



1 confinement strategy effectively suppresses shuttling, supports high sulfur loading, and ensures  
2 strong conductivity and lithium polysulfide adsorption for improved performance. The polar amine  
3 sites of the PDA layer enable strong chemical adsorption of polysulfides, localizing them on the  
4 electrode surface. Additionally, the PDA enhances electrolyte wetting, uptake, and ionic  
5 conductivity, improving  $\text{Li}^+$  transport. Figure 12d shows the CV curves of the S@Mxe@PDA  
6 cathode at  $0.2 \text{ mV s}^{-1}$ , with reduction peaks at 2.27 and 1.98 V corresponding to the formation of  
7  $\text{Li}_2\text{Sx}$  and  $\text{Li}_2\text{S}_2/\text{Li}_2\text{S}$ . Figure 12e displays long-term cycling stability at  $0.2 \text{ C}$ , with  
8 S@Mxe@PDA achieving  $1044 \text{ mAh g}^{-1}$  after 150 cycles (73% retention), outperforming S@Mxe  
9 ( $565 \text{ mAh g}^{-1}$ , 39% retention) due to better polysulfide confinement. Figure 12e,f demonstrates  
10 the rate performance of S@Mxe@PDA, showing stable capacities at  $1349\text{--}624 \text{ mAh g}^{-1}$  from  $0.2$   
11 to  $6 \text{ C}$ , with minimal capacity loss when returning to lower rates, indicating fast kinetics and  
12 stability.

13 Besides these, MXene-polymer hybrids can also be utilized for all-solid-state batteries and fuel  
14 cells<sup>19, 205, 257, 258</sup>.

## 15 **7.2 MXene-polymer nanocomposites in sensors and flexible electronics**

16 MXene-polymer nanocomposites offer several advantages over MXene-only systems in the field  
17 of sensors<sup>32, 60, 259, 260</sup>. The incorporation of polymers in MXene-based sensors can improve the  
18 sensing performance by enhancing selectivity, flexibility, sensitivity, and response time depending  
19 upon their sensing nature<sup>261–263</sup>. Polymers can provide a selective environment for target analytes  
20 by interacting with specific molecules, gases, or ions<sup>264, 265</sup>. The integration of MXene-polymer  
21 nanocomposites has shown significant promise in enhancing the performance of pressure and gas  
22 sensors due to the higher conductivity and surface area of MXenes. In a study, a bioinspired  
23 interlocked structure was developed to achieve high deformability in 2D MXene/natural  
24 microcapsule-based flexible pressure sensors using polyimide (PI) and PDMS<sup>262</sup>. To prepare  $\text{Ti}_3\text{C}_2$   
25 MXene/natural microcapsule nanofilm, a  $0.2 \text{ g}$  portion of natural microcapsule (NMC) was  
26 dispersed in  $10 \text{ mL}$  of ethanol to create a well-mixed solution.  $10 \text{ ml}$  of  $\text{Ti}_3\text{C}_2$  MXene solution was  
27 then added to the NMC solution, and the mixture was stirred for 2 hours to ensure uniform  
28 dispersion of  $\text{Ti}_3\text{C}_2$  MXenes and NMC. The mixture was subsequently filtered through a  
29 polypropylene membrane to create a composite film. This film was air-dried for 30 minutes at



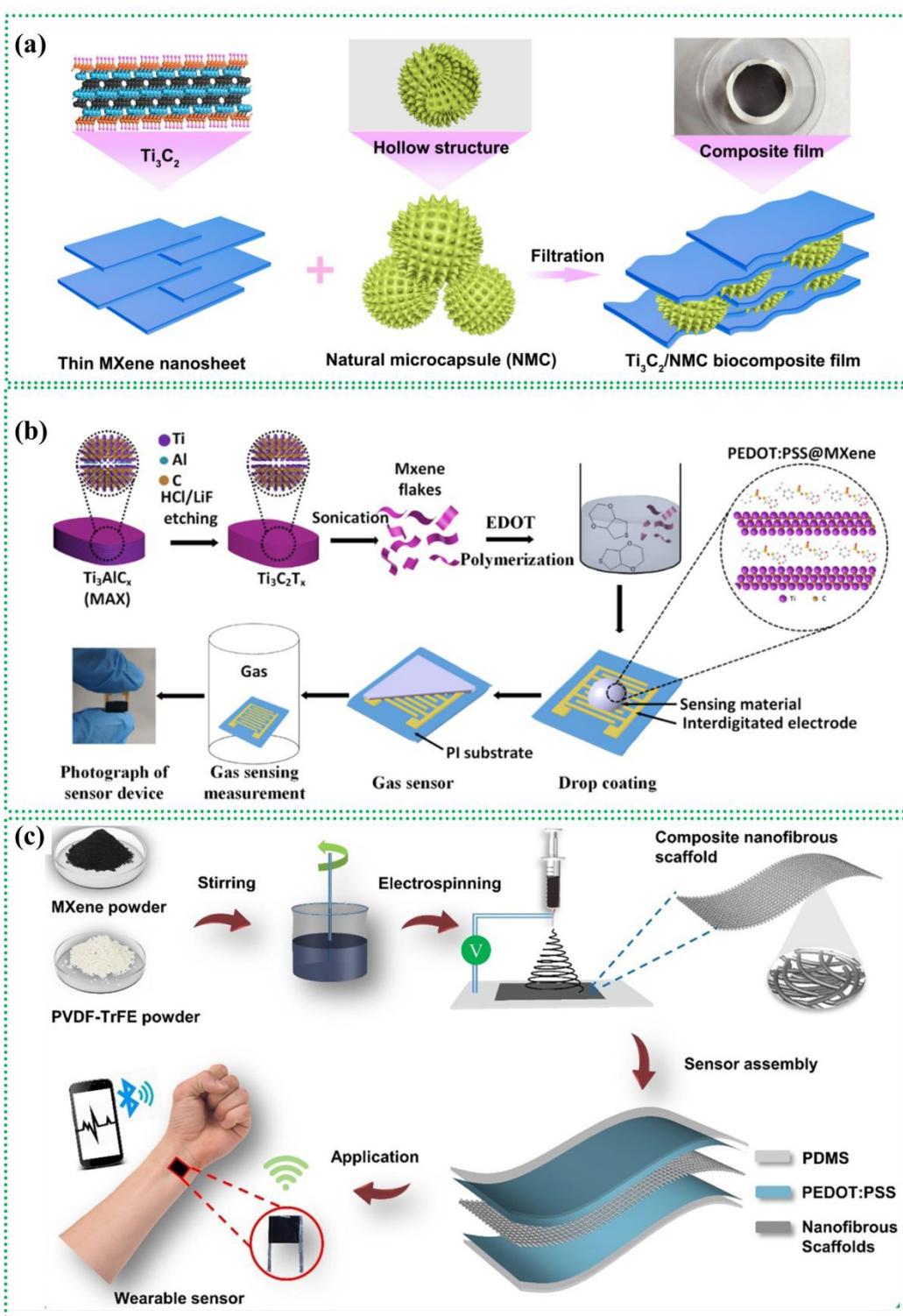
1 room temperature and carefully peeled off from the polypropylene membrane, resulting in a  
2 flexible  $\text{Ti}_3\text{C}_2\text{NMC}$  composite film (Figure 13a).

3 Polymeric  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene nanocomposites have exhibited promising applications in room-  
4 temperature ammonia gas sensing<sup>265</sup>. The PEDOT: PSS/MXene composites were prepared via a  
5 simple in situ polymerization process in/on  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene and subsequently utilized to fabricate  
6 a gas sensor on a PI substrate. The synthesis involved adding EDOT to the appropriate amount of  
7  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene suspension, followed by the introduction of ammonium persulfate (APS) and  
8 poly(4-styrene sulfonate) (PSS). The mixture was stirred for 24 hours at room temperature and  
9 1000 rpm, producing a black PEDOT: PSS/MXene composite solution (Figure 13b). These  
10 MXene-polymer nanocomposites are used to create wearable capacitive pressure sensors, with  
11  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene and poly(vinylidene fluoride-trifluoro ethylene) (PVDF-TrFE) as the dielectric  
12 layer between PEDOT: PSS and polydimethylsiloxane electrodes, facilitating reliable human  
13 physiological signal acquisition<sup>261</sup>. MXene powder in DMF was sonicated for 1 hour to form a  
14 homogeneous suspension, mixed with PVDF-TrFE to create a solution with up to 13 wt % MXene,  
15 and electro-spun into nanofibers. For the sensor, PDMS was spin-coated and cured on glass,  
16 followed by PEDOT: PSS spin-coating and DMSO treatment. The PEDOT: PSS film was peeled  
17 off, with CNS placed between two PEDOT: PSS layers, and carbon tape electrodes added (Figure  
18 13c).

19 Self-healing sensors based on MXene-polymer nanocomposites have attracted significant attention  
20 due to their unique capabilities in autonomously repairing damage and restoring functionality<sup>266</sup>.  
21 Polymers provide flexibility and conformability to MXene-based sensors, enabling their  
22 integration into various form factors and substrates. These composites combine the exceptional  
23 properties of MXene, such as high electrical conductivity and mechanical strength, with the self-  
24 healing properties of polymers<sup>267</sup>. A study recently developed a conductive MXene nanocomposite  
25 hydrogel with healable and degradable properties for advanced epidermal sensors<sup>267</sup>. The hydrogel  
26 was created by combining MXene, poly(acrylic acid) (PAA), and amorphous calcium carbonate  
27 (ACC). In the synthesis, PAA and calcium chloride were dissolved in water and stirred, followed  
28 by the addition of an MXene solution. A carbonate solution was then added, forming the MXene-  
29 PAA-ACC hydrogel. After formation, the hydrogel was washed thoroughly until the water was  
30 clear.

31





1  
2 **Figure 13.** MXene-polymer nanocomposites-based sensors. (a) Schematic diagram illustrating the  
3 fabrication process of the  $\text{Ti}_3\text{C}_2/\text{NMC}$  bio-composite film. Reproduced with permission from  
4 ref.<sup>262</sup>. Copyright 2019, American Chemical Society. (b) The schematic illustration depicts the  
5 synthesis process of PEDOT: PSS/MXene composites and the subsequent fabrication process of  
6 the gas sensor based on these composites. Reproduced with permission from ref.<sup>265</sup>. Copyright  
7 2020, American Chemical Society. (c) Schematic diagram illustrating the fabrication process of

1 the composite nanofiber scaffolds (CNS)-based pressure sensor. Reproduced with permission from  
 2 ref.<sup>261</sup>. Copyright 2020, American Chemical Society.

3 Besides these, there are many other reports on MXene-polymer composites given in Table 6 with  
 4 diverse applications<sup>32, 243, 260, 268</sup>.

5 Table 6. The comparison of several MXene-based composites as sensors.

6

| Sr. | Components   | MXene contents (wt.%) | Fabrication technique  | Structure type   | Sensor type            | Mechanical strength | Gauze factor              | Ref.           |
|-----|--|-----------------------|------------------------|------------------|------------------------|---------------------|---------------------------|----------------|
| 1   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PDMAEMA   | 78                    | Surface modification   | Accordion        | Temperature            | -                   | -                         | <sup>269</sup> |
| 2   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /Poly(N-isopropylacrylamide)/Polyacrylamide                | -                     | In situ polymerization | Porous network   | Temperature and Strain | 0.4 MPa             | -                         | <sup>270</sup> |
| 3   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PDADMA/BPEI   | 90.7                  | Physical mixing        | Layer-by-layer   | pH                     | -                   | 116 kΩ pH <sup>-1</sup>   | <sup>271</sup> |
| 4   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PEDOT/PVDF  | 5                     | In situ polymerization | Sandwich         | Pressure               | -                   | 0.51 kPa <sup>-1</sup>    | <sup>261</sup> |
| 5   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PVA/PDMS  | 0.2                   | Physical mixing        | Sandwich         | Pressure               | -                   | 1.5 kPa <sup>-1</sup>     | <sup>272</sup> |
| 6   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PVDF-TrFE   | 38                    | Physical mixing        | Sandwich         | Pressure               | -                   | 2213.68 kPa <sup>-1</sup> | <sup>273</sup> |
| 7   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PDA/AgNWs   | 16.7                  | Physical mixing        | Brick-and-mortar | strain                 | -                   | 200                       | <sup>274</sup> |
| 8   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PVA/Poly(vinylpyrrolidone)                                | 1                     | Physical mixing        | Porous network   | strain                 | 300 kPa             | 19.18                     | <sup>275</sup> |
| 9   | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /Poly(acrylic acid)(PAA)/Amorphous calcium carbonate (ACC) | 0.07                  | Physical mixing        | Porous network   | strain                 | 180 kPa             | 10.79                     | <sup>276</sup> |
| 10  | Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> /PAA   | 2                     | Physical mixing        | Porous network   | strain                 | 30 kPa              | 0                         | <sup>277</sup> |

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8

9

1 MXene-polymer composites can lead to the development of flexible electronic devices having  
2 lightweight, flexible, and high-performance devices with enhanced mechanical properties, tailored  
3 electrical conductivity, and improved protection against environmental factors<sup>16, 59</sup>. The  
4 synergistic effects between MXenes and polymers can be used in next-generation flexible  
5 electronic devices with diverse applications, including wearable electronics, flexible displays, EMI  
6 shielding, conformable sensors, and piezoelectric applications<sup>50, 60, 278, 279, 280, 281</sup>. Zhang et al.  
7 investigated a flexible MXene-decorated fabric (M-CF) featuring interwoven conductive  
8 networks. The study explored the fabric's multifunctional capabilities, specifically focusing on  
9 integrated Joule heating, electromagnetic interference shielding, and strain-sensing  
10 performances<sup>59</sup>. By incorporating MXene into the fabric's structure, the researchers aimed to  
11 enhance its electrical and thermal properties, making it a versatile material for various applications  
12 related to heating, shielding, and sensing. After etching the MXene inks were uniformly sprayed  
13 onto the surface of pretreated cotton fabrics (Figure 14a). To achieve different loading contents of  
14 MXene on the fabric, they adjusted the spray-drying cycles. By varying the MXene content in the  
15 cotton fabric, they aimed to optimize and find the most suitable MXene loading for achieving the  
16 desired multifunctional applications like EMI shielding, Joule heating, sensing, etc. (Figure 14b).  
17 The EMI shielding properties of the samples were studied within a frequency range of 8-12 GHz,  
18 employing a waveguide method. The average EMI shielding effectiveness of the 2 wt% MXene-  
19 based sample is ~25 dB, while for the 4 and 6 wt.%, it measured 33 and 36 dB, respectively. The  
20 sensors based on 2 wt% MXene led to maximum resistance change under the same bending strain,  
21 making the nanocomposite ideal for detecting small human activities. The optimized 2 wt.% M-  
22 CF sensor maintained consistent resistance change for more than 5000 cycles of bending and  
23 releasing. Attached to a finger, the MXene-based sensor consistently detected resistance changes  
24 during bending movements and accurately recorded a pulse rate of 80 beats per minute.

25 Polymer lamination can effectively mitigate MXene oxidation as evidenced by their application in  
26 various devices. Lee et al. demonstrated that laminating a thin poly(4-vinylphenol) (PVPh) layer  
27 as a protective film on MXene (PL-MXene) protects it from the external environment<sup>50</sup>. This  
28 combination was utilized for the electroluminescent (EL) display whose structure is demonstrated  
29 in Figure 14(c). The relative luminance variance ( $\Delta L/L_0$ ) of devices with PL-MXene and bare  
30 MXene electrodes over time is shown in Figure 14(d). Besides these, there are many other reports



1 on the usage of MXene-polymers nanocomposites in the domain of flexible devices with a wide  
2 variety of applications<sup>244, 248, 256, 258, 279, 282, 283</sup>.

3 MXene-polymer nanocomposites are also studied for piezoelectric applications. Piezoelectric  
4 sensors can transform the plentiful mechanical energy that surrounds us into electrical energy,  
5 mechanical energy harvesters are seen to be one of the most appealing energy harvesting  
6 technologies. Nevertheless, their poor electrical performance is preventing it from being used  
7 practically. Because the electrical performance of the energy harvester may be enhanced by  
8 harvesting the applied mechanical energy in two harvesters concurrently, hybridization of the two  
9 distinct mechanical energy harvesters such as MXene and any other piezoelectric material may  
10 offer a solution to this problem.

11 An overall schematic representation of the hybridization generator integrating MXene and barium  
12 titanate as conductive fillers in the PDMS matrix (HG-MBP) is shown in Figure 14e<sup>284</sup>. The HG-  
13 MBP was made of MXene/BaTiO<sub>3</sub>, polyimide (PI), and aluminum (Al), as seen in Figure 14e.  
14 The electrode, substrate, piezoelectric layer, and triboelectric layer are all PDMS (MBP) composite  
15 films. As seen in the inset photographic image of Figure 14e, the superior flexibility of HG-MBP  
16 was verified with a high bending angle using a bending test. This resulted from the intrinsic  
17 property of the MBP composite film, which has a thickness of  $125 \pm 10 \mu\text{m}$  and contains 2D and  
18 nano-scaled materials, such as MXene sheets and BaTiO<sub>3</sub> nanoparticles, inside the PDMS matrix  
19 with high elasticity. Schematic of MXene is shown in Figure 14g (i). Additionally, an X-ray  
20 diffraction (XRD) examination was performed to verify that MXene was successfully synthesized.  
21 As shown in Figure 14g (ii). A high open-circuit voltage of 80 V, a short-circuit current of 14  $\mu\text{A}$ ,  
22 and a power density of  $13.5 \text{ W/m}^2$  were achieved after determining the ideal MXene concentration.  
23 An example of this is the successful control of a 3D printer-modeled robot hand using the finger  
24 joint motions of a real hand that has HG-MBPs attached. The k-mean clustering approach was also  
25 used in the development of the object recognition system, which distinguishes between various  
26 materials with a high classification accuracy of 93.33%. These findings demonstrate the great  
27 potential of the suggested HG-MBP as a material detection sensor and human gesture manipulation  
28 system, which is anticipated to be used as a next-generation e-skin in the human-machine interface.  
29 MXene exhibits a better piezoelectric effect on poly(vinylidene fluoride-co-trifluoroethylene)  
30 (PVDF-TrFE) compared to polyvinylidene fluoride (PVDF). Generally (beta-phase)  $\beta$ -phase in  
31 PVDF crystals exhibit the best piezoelectric properties, although achieving this phase in PVDF is



1 still challenging<sup>285 286</sup>. However, PVDF-TrFE inherently possesses a larger content of the  
2 electroactive  $\beta$ -phase than PVDF due to its higher steric hindrance<sup>287</sup>. The incorporation of MXene  
3 into PVDF-TrFE further promotes the nucleation of this phase, leading to improved piezoelectric  
4 properties<sup>288</sup>. This enhancement is less significant in PVDF due to its lower initial  $\beta$ -phase content.  
5 The dielectric constant is significantly increased, and dielectric loss is decreased in PVDF-TrFE  
6 as a result of the interaction between the polymer matrix and the surface functional groups of  
7 MXene. PVDF-TrFE/MXene composites exhibit enhanced mechanical flexibility and durability,  
8 making them more suitable for applications in flexible electronics and wearable devices. Fatemeh  
9 M. et al.<sup>288</sup> reported the fabrication of acoustic energy harvesters using electrospinning of the  
10 piezoelectric polymer PVDF-TrFE onto fabric-based electrodes. The incorporation of  $Ti_3C_2T_x$   
11 MXene flakes effectively induced polarization locking within the electro-spun PVDF-TrFE,  
12 optimizing its electromechanical performance. The resulting device was mechanically robust,  
13 lightweight, and flexible, enabling efficient energy harvesting and sound detection within the 50  
14 to 1000 Hz frequency range and at sound pressure levels between 60 and 95 dB. The device  
15 demonstrated an impressive sensitivity of  $37 \text{ VPa}^{-1}$ , outperforming previous PVDF-based acoustic  
16 harvesters. It achieved a peak output power of  $19 \text{ mW/cm}^3$  at 200 Hz and 95 dB. This advancement  
17 highlights the potential of MXene-enhanced PVDF-TrFE composites in powering small electronic  
18 devices, including implantable biomedical devices, smart wearables, and remote Internet-of-things  
19 (IoT) systems. The comparison of PVDF/MXene and PVDF-TrFE/MXene composites is given in  
20 Table 7. Numerous studies that reported the applications of PVDF-TrFE/MXene-based  
21 piezoelectric nanogenerators can be found here<sup>289 290 291 292</sup>.

22

23

24



1 Table 7. The comparison of several MXene-based composites as piezoelectric nanogenerators.

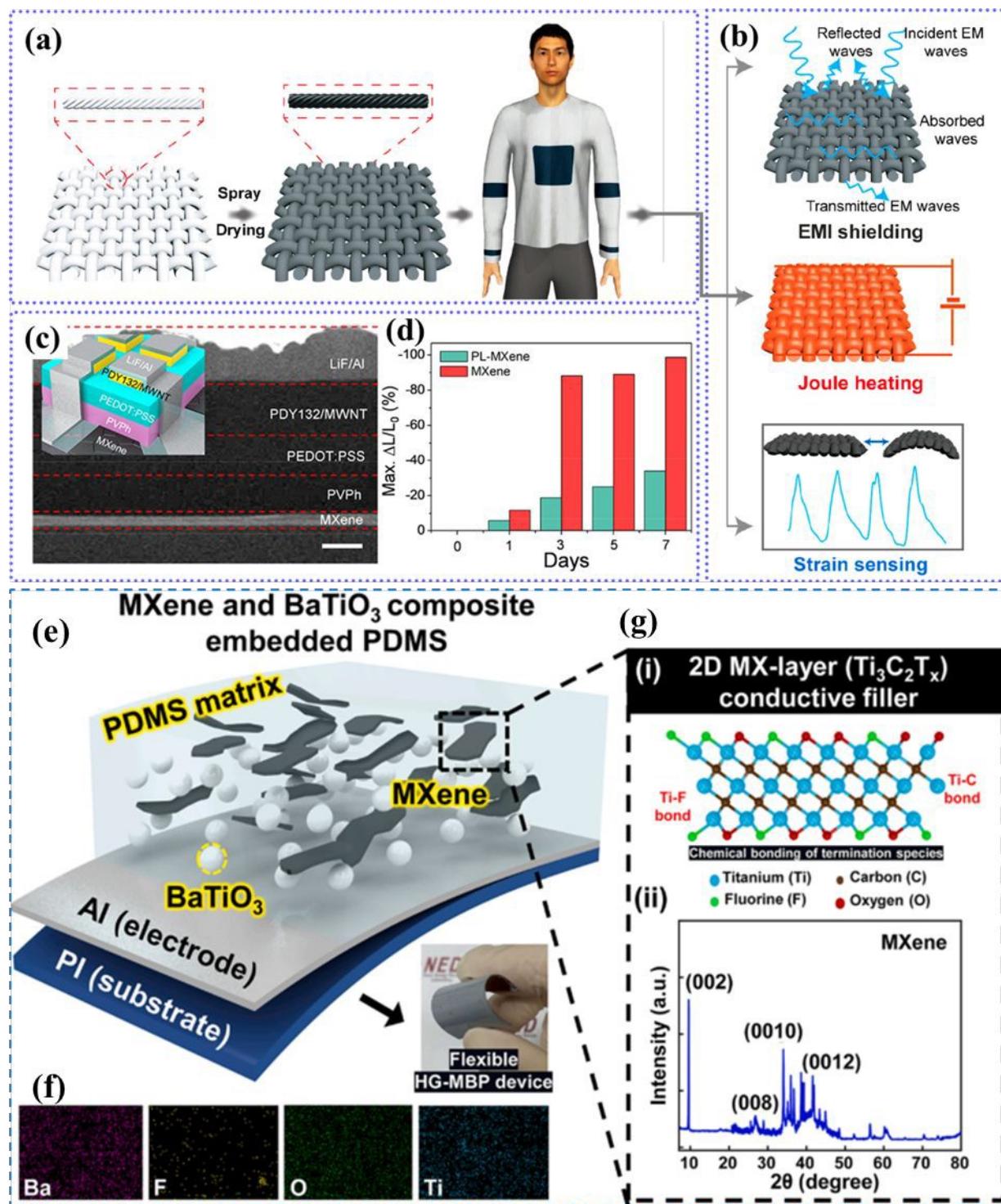
| Components  | MXene contents (wt.%)         | Device dimensions        | Source                   | Fabrication technique   | Sensitivity                 | Power density              | Ref.           |
|---|-------------------------------|--------------------------|--------------------------|-------------------------|-----------------------------|----------------------------|----------------|
| PVA/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>       | -                             | 8 × 8 mm <sup>2</sup>    | 0.5 H                    | Electrospinning         | -                           | 42 mW m <sup>-2</sup>      | <sup>293</sup> |
| Glycine/Nb <sub>2</sub> C T <sub>x</sub>                | -                             | 100 mm <sup>2</sup>      | 0.6 Hz,<br>10 N          | Crystallization         | 5 pC N <sup>-1</sup>        | -                          | <sup>294</sup> |
| PVDF/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>      | -                             | 1 × 1 cm <sup>2</sup>    | 96.5 d<br>B,<br>0.2 N    | Crystallization         | 0.4 nA<br>kPa <sup>-1</sup> | -                          | <sup>295</sup> |
| PVDF/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>      | 0.4wt.%                       | 2.5 cm ×<br>3.0 cm       | 1–3 Hz                   | Electrospinning         | 43 pCN <sup>-1</sup>        | -                          | <sup>281</sup> |
| PVDF/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>      | 1.0 wt.%                      | 2 × 20 mm                | 1–<br>10 <sup>7</sup> Hz | Microinjection Molding  |                             | 18.9<br>μWcm <sup>-2</sup> | <sup>280</sup> |
| PVDF/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>      | 0.01-0.05<br>g/L              | 2 cm × 2<br>cm           | 4.7 N,<br>5 Hz           | Spin- and spray-coating | -                           | 14 μWcm <sup>-2</sup>      | <sup>296</sup> |
| PVDF/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>      | 5-25 wt%                      | 20 mm × 20<br>mm         | 1-8 Hz                   | Electrospinning         | -                           | 11.213 Wm <sup>-2</sup>    | <sup>297</sup> |
| PVDF/CNT/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub>  | 0.05-0.2<br>wt %              | 2 × 1.5 cm <sup>2</sup>  | 1–500<br>MΩ              | Electrospinning         | -                           | 18.08 W m <sup>-2</sup>    | <sup>298</sup> |
| PVDF-TrFE/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 0.05- 0.2<br>wt% <sup>2</sup> | 12.56 cm <sup>2</sup>    | 200<br>Hz,<br>95 dB      | Electrospinning         | 37 V Pa <sup>-1</sup>       | 0.207<br>mWm <sup>-2</sup> | <sup>288</sup> |
| PVDF-TrFE/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 0.02-0.5<br>wt.%              | 2.4 cm <sup>2</sup>      | 5 kPa,<br>1 Hz           | Printing                | -52.0<br>pC N <sup>-1</sup> | -                          | <sup>299</sup> |
| PVDF-TrFE/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 2.0 wt%                       | 1 × 1<br>cm <sup>2</sup> | 20 N,<br>1 Hz            | Electrospinning         | -                           | 3.64 mWm <sup>-2</sup>     | <sup>285</sup> |
| PVDF-TrFE/Ti <sub>3</sub> C <sub>2</sub> T <sub>x</sub> | 16% (w/v)                     | 15 × 1.3 mm              | 7 N, 6<br>Hz             | Electrospinning         | -                           | 4.02 W/m <sup>2</sup>      | <sup>289</sup> |

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4 **Figure 14.** MXene-polymer nanocomposites in flexible electronics. (a). Multifunctional MXene-decorated cotton woven fabrics fabricated by employing the spray-coating method, where the MXene material is applied to the cotton woven fabric to impart its multifunctional properties like



1 EMI shielding, Joule heating and strain sensing, etc. (b) Demonstration indicating the applications  
2 of MXene coated flexible fabrics in different areas. Reproduced with permission from ref.<sup>59</sup>.  
3 Copyright 2020, American Chemical Society. (c) SEM image showing the cross-sectional view of  
4 an organic AC-EL display with a PL-MXene electrode (scale bar: 50 nm). The inset provides a  
5 schematic representation of the PL-MXene organic AC-EL display. (d) Maximum  $\Delta L$  (luminance  
6 change) to  $L_0$  (initial luminance) ratio of bare MXene and PL-MXene organic AC-EL displays as  
7 a function of air exposure duration (days). <sup>50</sup>. Copyright 2020, American Chemical Society. (e)  
8 General schematic representation of the manufactured HG-MBP with the Al electrode connected  
9 to the PI substrate spin-coated with MBP composite film. The inset graphic illustrates the  
10 constructed HG-BMP's flexibility. (f) MXene and BaTiO<sub>3</sub> particles implanted in the PDMS matrix  
11 as shown in a cross-sectional EDX picture. (g) (i) MXene's schematic chemical bond structure and  
12 (ii) XRD result <sup>284</sup>.

13 Zhao and colleagues used rolling <sup>281</sup>, hot pressing, and electrospinning techniques to create a high-  
14 performance MXene/PVDF composite film with a  $\beta$ -phase of more than 95 weight percent. The  
15 MXene/PVDF-based sensor showed exceptional voltage sensitivity, up to 0.0480 V N<sup>-1</sup>. It is  
16 important to remember that the MXene used in this work was generated via HF etching, which left  
17 it with rich surface groups. The favorable impact may be primarily ascribed to the hydrogen  
18 bonding interaction that favors all trans planar conformation ( $\beta$ -phase) during PVDF  
19 crystallization and is brought about by the –OH groups of the MXene and F atoms of PVDF chains.  
20 The directed distribution and regular stack of MXene flakes, which facilitated the transfer, storage,  
21 and release of electric charge, were further examined by Han and colleagues <sup>280</sup>. Furthermore, this  
22 paper mentioned the -F groups of the MXene with interfacial compatibility, which are typically  
23 thought of as a type of significant surface group.

24 Even though adding MXenes to composites increases their piezoelectricity for improved sensing  
25 properties, if the MXene level is over the percolation threshold, the composite's performance  
26 drastically declines <sup>300,301</sup>. This may be explained by the fact that when the amount of conductive  
27 MXene is too high, many connections are created that degrade the performance. Increased MXene  
28 content may result in additional  $\beta$  phases but a conductive route inside the composite. Additionally,  
29 a lower MXene content results in fewer  $\beta$  phases. One important component for improving  
30 performance is the percolation threshold. Li and colleagues used molecular dynamics to simulate  
31 MXene/PVDF composite material systems with varying MXene levels based on the Forceite model  
32 <sup>302</sup>. They then computed the free volume fraction (FFV) to demonstrate the impact of MXene  
33 sheets. On the shape of the macromolecular chain. The space between molecules is known as free  
34 volume. When a suitable quantity of MXene sheets was introduced into the PVDF polymer system,



the polymer system's FFV dropped to its lowest value, indicating that there was less room for macromolecular chains to move. Additionally, the optimized sensor demonstrated a sensitivity of up to  $55.42 \text{ mV kPa}^{-1}$ .

Due to their varied inherent characteristics, MXenes give composite materials new functions in addition to improving piezoelectric performance. In addition to their electrical benefits, MXenes are biocompatible, which makes them appropriate for a range of biomedical applications<sup>303, 304, 304</sup>. MXene-based composites can be employed safely in settings that call for interactions with biological systems thanks to their biocompatibility. MXenes is a promising material for advanced composite technologies because of its improved piezoelectricity and bio-friendly qualities, which help to close the gap between high-performance materials environmentally, and biologically compatible solutions. By using MXenes' high electrical conductivity to increase electron transfer rates, Fu and colleagues were able to generate and transport electrical charges under mechanical stress, improving the piezoelectric response<sup>305</sup>. Furthermore, the composite's MXenes not only generated sufficient heat to eradicate bacteria while simultaneously producing singlet oxygen, which may also have a highly effective sterilizing effect. This suggests that it has a lot of promises for use in biomedical and self-powered body monitoring applications. Comparison of several MXene-polymer composites in field of piezoelectric nanogenerators is given in Table 7.

### 7.3 MXene-polymer nanocomposites in 3D/4D printing

MXene polymer composites offer great promise for 3D/4D printing applications, integrating MXene's exceptional properties of high electrical conductivity and mechanical strength with the versatility and tunability of polymers<sup>26, 64, 306</sup>. Enabled by 3D/4D printing technology, these composites showcase dynamic and shape-changing capabilities in response to external stimuli, paving the way for advanced engineering and smart applications<sup>307, 308</sup>.

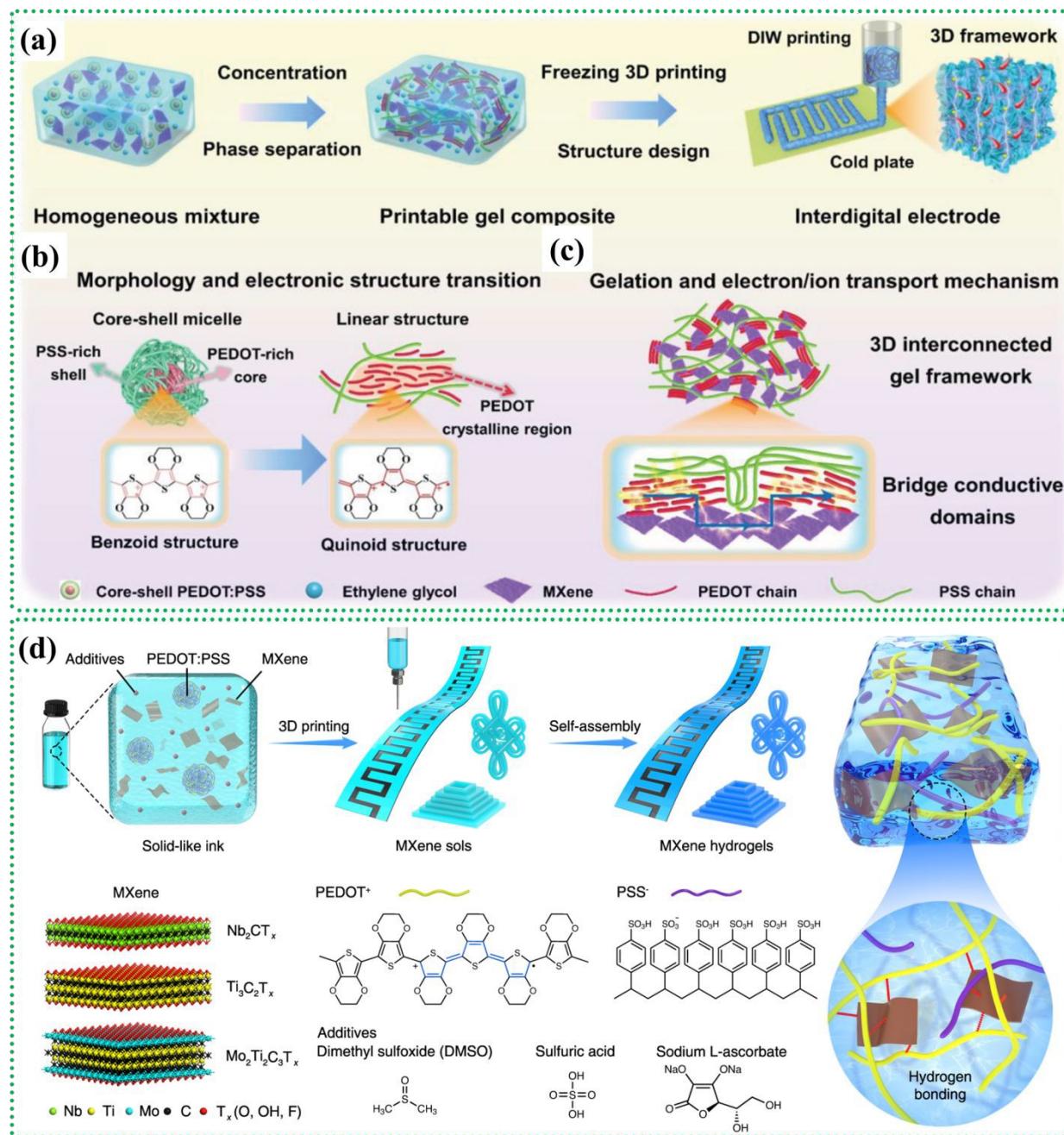
The programmable micro-supercapacitors can be developed using 3D printing of composite ink consisting of PEDOT: PSS/MXene/ethylene glycols (PME)<sup>26</sup>. In Figure 15a, the design and preparation procedure of 3D printed PME gel composites for micro-supercapacitors is illustrated. By mixing MXene and ethylene glycol (EG), and PEDOT: PSS solution an ink was prepared. During the fabrication process, the ink was transferred to a syringe and extruded under pressure through a needle to construct thick interdigitated electrodes for the MSCs. To achieve controlled solidification and form a 3D highly interconnected framework, a freezing technology utilizing a



1 cold plate was applied during the printing process. In this process PEDOT: PSS (Figure 15b) plays  
2 a significant role, and by appropriately bridging the PEDOT structures an integrated porous  
3 structure is created for the optimization of ion/electron transport kinetics in the fabricated gel  
4 (Figure 15c).

5 In addition to the development of 3D printing, the development of 4D printed hydrogels using  
6 MXene and PEDOT: PSS, showcasing high-efficiency pseudocapacitive energy storage  
7 capabilities<sup>309</sup>.





1 MXene hydrogels were prepared via self-assembly by mixing  $Ti_3C_2T_x$  MXene suspension with  
2 PEDOT suspension, followed by sonication. A solution containing DMSO, sulfuric acid, sodium  
3 L-ascorbate, and deionized water was added and stirred. The mixture was then poured into molds  
4 and heated to form  $Ti_3C_2T_x$  MXene hydrogels. These hydrogels were further treated with sulfuric  
5 acid to improve mechanical strength and washed to remove impurities. The optimization involved  
6 adjusting MXene content, DMSO volume, sulfuric acid concentration, and sodium L-ascorbate  
7 ratio. The method offers numerous advantages, especially its remarkable versatility and feasibility  
8 in synthesizing various MXenes such as  $Nb_2CT_x$ ,  $Ti_3C_2T_x$ , and  $Mo_2Ti_2C_3T_x$ .

9 An approach to 3D printing using MXene and poly(vinyl alcohol) (PVA) composites using  
10 MXene-surfactant ink has also been proposed for energy storage applications. Through the  
11 controlled deposition of highly conductive MXene particles onto a PVA matrix, the fabricated  
12 sample exhibited conductive behavior<sup>63</sup>. In a separate study, Li et al. demonstrated the production  
13 of elastic nanocomposites by encapsulating 3-(trimethoxysilyl)propyl methacrylate-modified  
14 MXene nanosheets within a photocurable polyurethane acrylate resin (PAR) matrix using digital  
15 light processing 3D printing. By adjusting the MXene content in the PAR, the mechanical  
16 properties of the elastomers were tailored. The resulting MXene-PAR nanocomposites, containing  
17 0.1% w/w fillers, exhibited remarkable tensile strength and elongation at a break of 23.3 MPa and  
18 404.3%, respectively, representing a significant increase of 100.8% and 37.8%, compared to the  
19 control<sup>310</sup>. Some other reports on MXene-polymer composites in 3D/4D printing are also available  
20 in the literature<sup>307, 311</sup>.

#### 21 **7.4 MXene-polymer nanocomposites in EMI shielding**

22 EMI shielding is the most explored area among the applications of MXene-polymer  
23 nanocomposites. These composites offer several advantages in the field of EMI shielding<sup>312, 313</sup>.  
24 MXene-polymer composites exhibit lightweight, conductivity, and improved mechanical  
25 properties making them highly suitable for EMI shielding applications<sup>313, 314</sup>. Polymers provide  
26 the advantage of tunability in MXene-polymer composites, allowing the customization of EMI  
27 shielding performance for specific applications or requirements<sup>29, 313</sup>. By selecting appropriate  
28 polymers with specific dielectric properties, the composite's overall electrical conductivity and  
29 impedance matching can be tailored to provide optimal shielding performance within desired  
30 frequency ranges<sup>29, 204</sup>. Polymers in MXene-polymer composites provide chemical resistance and

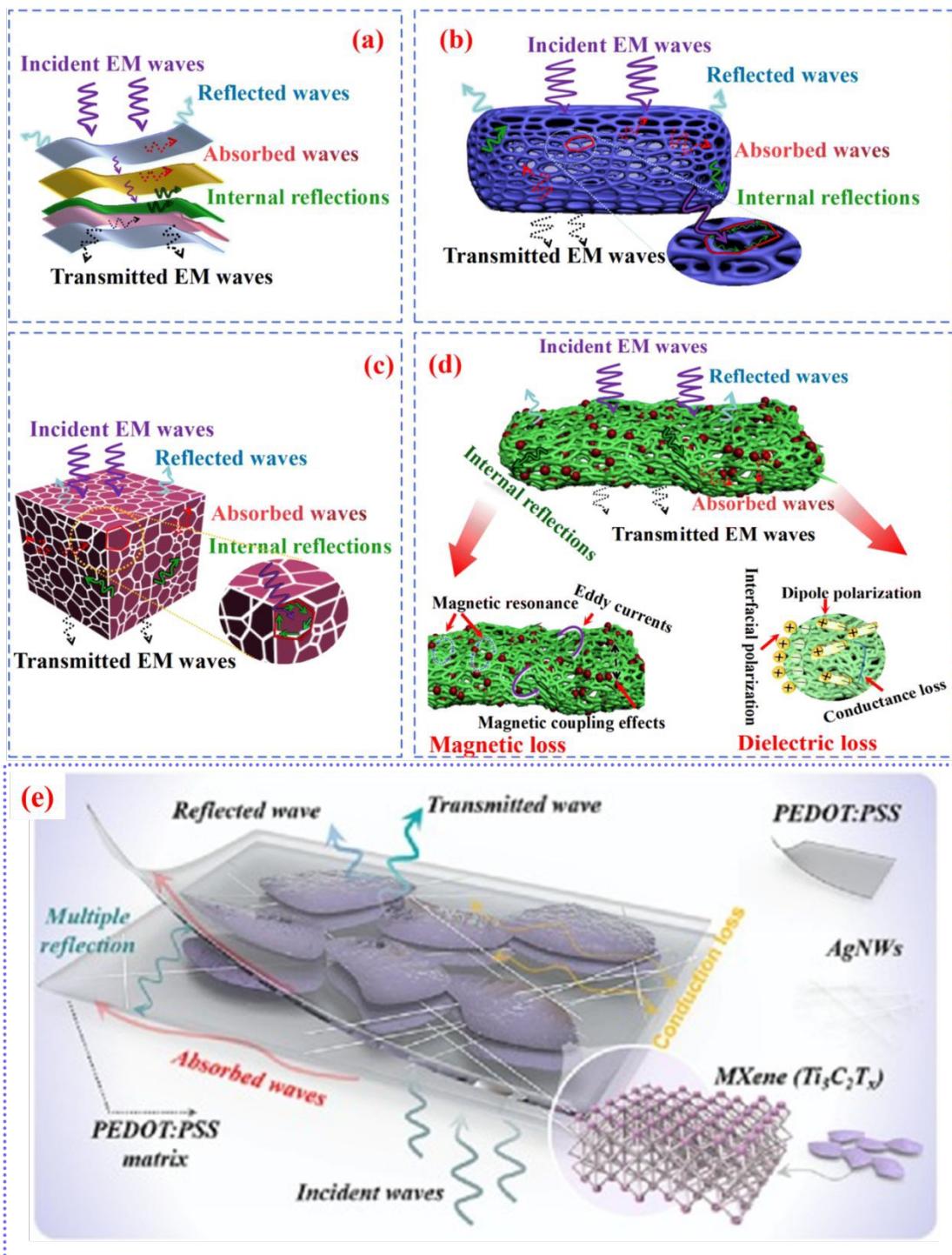


1 durability, enhancing the longevity and performance of EMI shielding materials. The polymer  
2 matrix acts as a protective layer, shielding the MXene flakes from environmental factors such as  
3 moisture, chemicals, or oxidation<sup>315</sup>.

4 Different structures of MXene/polymer composites offer distinct mechanisms for EMI shielding  
5 depending on various factors<sup>315</sup>. In multilayer MXene/polymer composites, multiple MXene layers  
6 are stacked within the polymer matrix (Figure 16a). The interlayer spacing and alignment influence  
7 the EMI shielding. Electromagnetic waves penetrate the composite and get reflected or scattered  
8 at the interfaces between the MXene layers and the polymer. This multiple reflection and scattering  
9 lead to effective EMI attenuation. Porous MXene/polymer composites have voids or pores within  
10 the material (Figure 16b). These voids can trap and dissipate electromagnetic waves, reducing their  
11 propagation. The interconnected porous network of MXene also enhances the electrical  
12 conductivity, further improving the EMI shielding efficiency. In segregated MXene/polymer  
13 composites, MXene and polymer phases exist as distinct domains within the material (16c). The  
14 MXene domains act as conductive pathways, while the polymer regions provide structural support.  
15 This phase separation enhances electrical conductivity and enables effective EMI shielding by  
16 creating a conductive network to dissipate electromagnetic energy. Some MXene/polymer  
17 composites include magnetic particles or other conductive additives (Figure 16d). MXene/polymer  
18 composites with conductive and magnetic fillers show excellent EMI-shielding performance. The  
19 conductive network inculcates an impedance mismatch at the composite/air interface, leading to a  
20 high reflection. Magnetic materials enhance impedance matching at the conductive filler/air  
21 interface, increasing EMW absorption. These additives enhance the electromagnetic absorption  
22 and scattering properties of the composite.

23 To address the challenges posed by harsh freezing and high-humidity environments for polymeric  
24 EMI shielding materials, Chang et al. developed ultrathin, flexible MXene/Ag nanowires/PEDOT:  
25 PSS composite coatings<sup>316</sup>. Fabricated via drop-casting and hydrophobic spraying, these coatings  
26 achieve an EMI shielding effectiveness of 31.5 dB at ~10 μm thickness. These nanocomposite  
27 coatings also offer excellent electro/photo-thermal properties, water repellency, interfacial  
28 adhesion, and mechanical durability, making them suitable for cold and damp conditions. The  
29 shielding mechanism of the MXene/AgNWs/PEDOT: PSS coating is shown in Figure 16(e).





**Figure 16.** EMI shielding mechanisms vary among different structures of MXene/polymer composites. (a) Multiple MXene layers lead to reflection and scattering, effectively attenuating EMI. (b) The interconnected MXene network and voids trap and dissipate electromagnetic waves, reducing their propagation. (c) Separate MXene and polymer domains create conductive pathways, ensuring efficient EMI shielding. (d) The inclusion of magnetic or conductive fillers enhances impedance matching, improving EMI absorption<sup>315</sup>. (e) Diagram depicting electromagnetic

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microwave dissipation in the MXene/AgNW/PEDOT:PSS coating. Reproduced with permission from ref.<sup>316</sup>. Copyright 2023, Elsevier Ltd.

As an electromagnetic wave strikes the MXene/AgNWs/PEDOT: PSS coating, most of it reflects due to impedance mismatch. The penetrating portion interacts with dense charge carriers, leading to significant polarization and conduction losses. The 1D AgNWs bridge the gaps between MXene nanosheets, creating conduction networks that enhance electron hopping and migration, thus increasing conduction losses. Additionally, the lamellar microstructures cause the wave to bounce between MXene layers, further dissipating energy due to impedance mismatch at the PEDOT: PSS/MXene interfaces.

In a recent study,  $Ti_3C_2T_x$  MXene composite films were developed for efficient EMI shielding, featuring photothermal healing, stretchability, and high conductivity<sup>211</sup>. By increasing the MXene content in the waterborne polyurethane (WPU), natural rubber, and MXene-based composite (WNM) composite films the conductivity increased sharply which led to the high EMI shielding for WNM composite exhibiting the EMI shielding efficiency (SE) of 76.1 dB at a thickness of  $336 \pm 15 \mu\text{m}$  for X-band, whereas, for Ku-band the EMI SE value is  $\sim 80$  dB. The EMI shielding mechanism in the composite films is based on induced polarization due to the MXene functional groups. The local dipoles between Ti and surface groups (-F and -OH), especially -F on MXene surfaces, induce dipole polarization, leading to attenuation of penetrated EMWs through interfacial polarization loss. Additionally, polarized interfaces between the honeycomb-like MXene network and the polymeric matrix enhance polarization loss, further improving EMI shielding performance. The honeycomb-like MXene network structure contributes to the exceptional EMI shielding performance of the WNM films across a wide frequency range.

These advantages of MXene-polymer composites in EMI shielding make them highly attractive for various industries, including flexible electronics<sup>317</sup>, telecommunications<sup>318</sup>, aerospace<sup>319</sup>, where effective protection against electromagnetic interference is crucial<sup>320</sup>. The synergistic effects between MXenes and polymers enable the development of lightweight, flexible, and high-performance EMI shielding materials with improved properties and capabilities.

## 7.5 MXene-polymers nanocomposites for anti-corrosion applications

The exceptional characteristics of  $Ti_3C_2T_x$ , such as its unique layered structure and large specific surface area, along with remarkable electrical and mechanical properties, make it highly promising

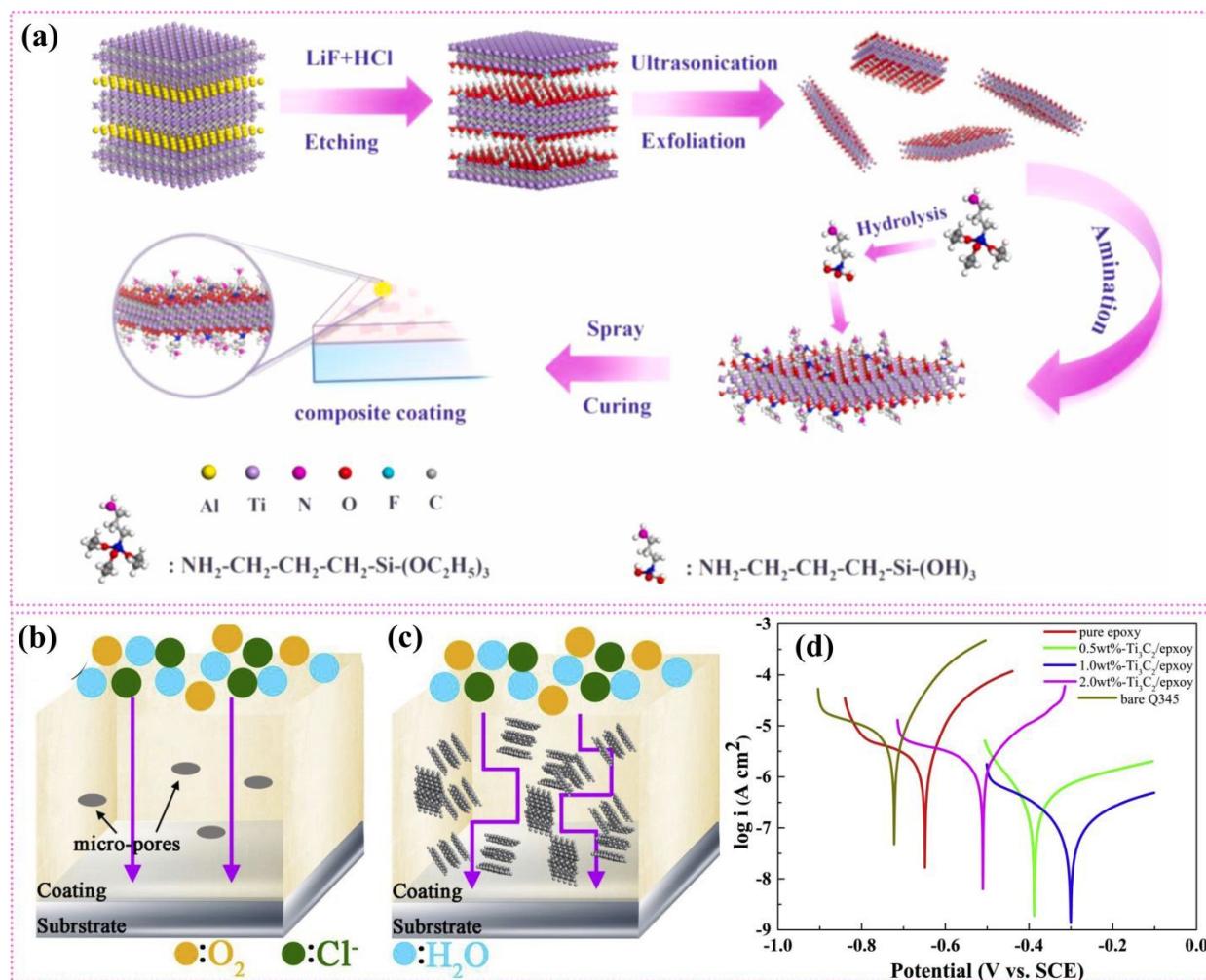
for anti-corrosion applications<sup>66, 321, 322</sup>. To utilize the inherent anticorrosion properties of pristine  $Ti_3C_2T_x$  nanosheets these were incorporated in the form of single- to few-layer  $Ti_3C_2Tx$  nanosheets into a waterborne epoxy coating (WEC) through a simple physical mixing. Zhang et al. conducted a study on the surface functionalization of  $Ti_3C_2T_x$  and its application in aqueous polymer nanocomposites to enhance corrosion protection<sup>322</sup>. In this approach, they utilized [3-(2-Aminoethyl) aminopropyl] trimethoxy silane (AEAPTES), a silane coupling agent, to modify the  $Ti_3C_2T_x$  MXene. This modification aimed at adjusting the wettability of  $Ti_3C_2T_x$  to improve its compatibility with the polymer matrix in the nanocomposites.

In another study, a few-layer amino-functionalized  $Ti_3C_2T_x$  nanosheets (k- $Ti_3C_2$ ) were combined with an interpenetrating polymer network (IPN) to create k- $Ti_3C_2$ /IPN composite coatings and examined the tribological characteristics of these coatings<sup>323</sup> (Figure 16a). The wear rates of the k- $Ti_3C_2$ -0.75 (0.75 wt.% amino functional  $Ti_3C_2T_x$ ) composite coating decreased by 82.41% before UV aging and 74.55% after UV aging, compared to the pure IPN coating, under dry friction conditions. Additionally, during the tribo-corrosion test in a 3.5 wt% NaCl solution, the k- $Ti_3C_2$ -0.75 composite coating exhibited the highest open circuit potential (OCP) and the lowest coefficient of friction (COF) among all coatings, both before and after UV aging.

In a recent study, the anticorrosion and anti-wear behavior of an inorganic-organic multilayer protection system consisting of an epoxy coating incorporating  $Ti_3C_2T_x$  MXene. The researchers designed and prepared this protective system to enhance its effectiveness against corrosion and wear<sup>66</sup>. The hydrophilic nature of  $Ti_3C_2T_x$  allowed it to maintain stable dispersions within the epoxy matrix. This characteristic played a vital role in creating an effective physical barrier for anti-corrosion purposes. The  $Ti_3C_2$ /epoxy coatings with different  $Ti_3C_2$  content (0.5, 1, and 2 wt. %  $Ti_3C_2T_x$ /epoxy) were obtained via the curing reaction of epoxy resin with an amine curing agent (Figure 17a). The mechanism of protection from corrosion with  $Ti_3C_2$  content was proposed as demonstrated in Figure 17b-c. With no MXene content the corrosion probability is high and as the MXene content is increased the corrosion inhibition efficiency increases. But as the  $Ti_3C_2$  content was raised to 2.0 wt. %, irregular corrosion particles began to accumulate once more and corrosion inhibition efficiency decreased. This indicates that beyond the optimal content, MXene tends to agglomerate, adversely impacting the anti-corrosion performance. Hence,  $Ti_3C_2$  nanosheets can effectively enhance the corrosion resistance of the coatings, but only when added in the optimal



amount. The Tafel plots display the corrosion behavior of the uncoated Q345 sample (polished steel), pure epoxy, and  $\text{Ti}_3\text{C}_2\text{T}_x$ /epoxy composites with different  $\text{Ti}_3\text{C}_2\text{T}_x$  ratios (Figure 17d).



**Figure 17.** The anti-corrosion performance of MXene-polymer composites. (a) Synthesis of k- $\text{Ti}_3\text{C}_2$ /IPN coatings. Reproduced with permission from ref.<sup>323</sup>. Copyright 2021, Elsevier Ltd. Schematic representation of the corrosion process in two scenarios: (b) Without  $\text{Ti}_3\text{C}_2$  contained epoxy coating and (c) With  $\text{Ti}_3\text{C}_2$  contained epoxy coating. (d) Tafel plots of the samples immersed in 3.5% NaCl for 96 hours. Among the uncoated and coated samples, the 1 wt. %-coated sample exhibited the most superior protection. This was evident from the substantial positive shift in potential value ( $E_{\text{corr}}$ ) and the lowest corrosion current ( $I_{\text{corr}}$ ). The potential was measured relative to the saturated calomel electrode, utilized as the reference electrode. Reproduced with permission from ref.<sup>66</sup>. Copyright 2019, Elsevier Ltd.

Following a 96-hour immersion in a 3.5% NaCl solution, it was observed that the  $\text{Ti}_3\text{C}_2\text{T}_x$  provided enhanced corrosion protection on the steel substrates compared to pure epoxy coatings. This improvement in anti-corrosion properties was attributed to MXene flakes in an optimized concentration, acting as thin film barriers that hindered the diffusion of electrolytes and provided

1 effective corrosion protection to the substrate. The anti-corrosion performance can also be  
2 achieved through well-dispersed MXene-polymer composite coatings, made possible by covalent  
3 modification and ambient electron-beam curing<sup>241</sup>.

#### 4 **7.6 MXene-polymers nanocomposites in biomedical applications**

5 Polymer-functionalized MXenes exhibit exceptional properties that make them highly valuable for  
6 various applications in the medical sector. The big advantage is that the polymers have better  
7 compatibility, hence these nanocomposites can also be applied to numerous biomedical  
8 applications<sup>282, 324</sup>. The applications include antimicrobial treatments, photothermal therapy (PTT),  
9 drug delivery systems, diagnostic imaging techniques, biosensors, and bone regeneration  
10 processes. MXene polymer nanocomposites have shown great promise in biomedical applications.  
11 These nanocomposites combine the unique properties of MXene materials, such as excellent  
12 conductivity, high surface area, and antibacterial activity, with the versatility and biocompatibility  
13 of polymers. They hold potential for various biomedical uses, including tissue engineering<sup>237, 325</sup>,  
14 cancer therapy<sup>326, 327, 328</sup>, drug delivery systems<sup>207, 329</sup>, biosensors<sup>330</sup>, and antimicrobial coatings<sup>331,</sup>  
15 <sup>332</sup>. MXene polymer nanocomposites offer exciting opportunities for advancing medical  
16 technologies and improving healthcare outcomes.

##### 17 **7.6.1 Antimicrobial applications**

18 The hydrophilic nature and anionic surface properties of MXenes enhance their interaction with  
19 bacterial cell membranes. Through hydrogen bonding, the functional groups of MXenes interact  
20 with lipopolysaccharide molecules on the cell membrane, leading to cell inactivation. This  
21 interaction hinders nutrient intake, effectively inhibiting bacterial growth. Additionally, the  
22 formation of a conductive bridge over the lipid bilayer facilitates the transfer of reactive electrons  
23 from the bacterial cell to the external environment, ultimately causing cell death<sup>74, 75</sup>. The  
24 application of Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>, a high aspect ratio material, as a coating on PVDF membranes resulted in  
25 notable improvements in hydrophilicity, as evidenced by a reduced contact angle of 37°.  
26 Additionally, the presence of large pores in the membrane was mitigated. As a result, the viability  
27 and growth of *E. coli* (Gram-negative bacteria) were reduced by approximately 73%, while *B.*  
28 *subtilis* (Gram-positive bacteria) experienced a growth inhibition of around 67%<sup>74</sup>.

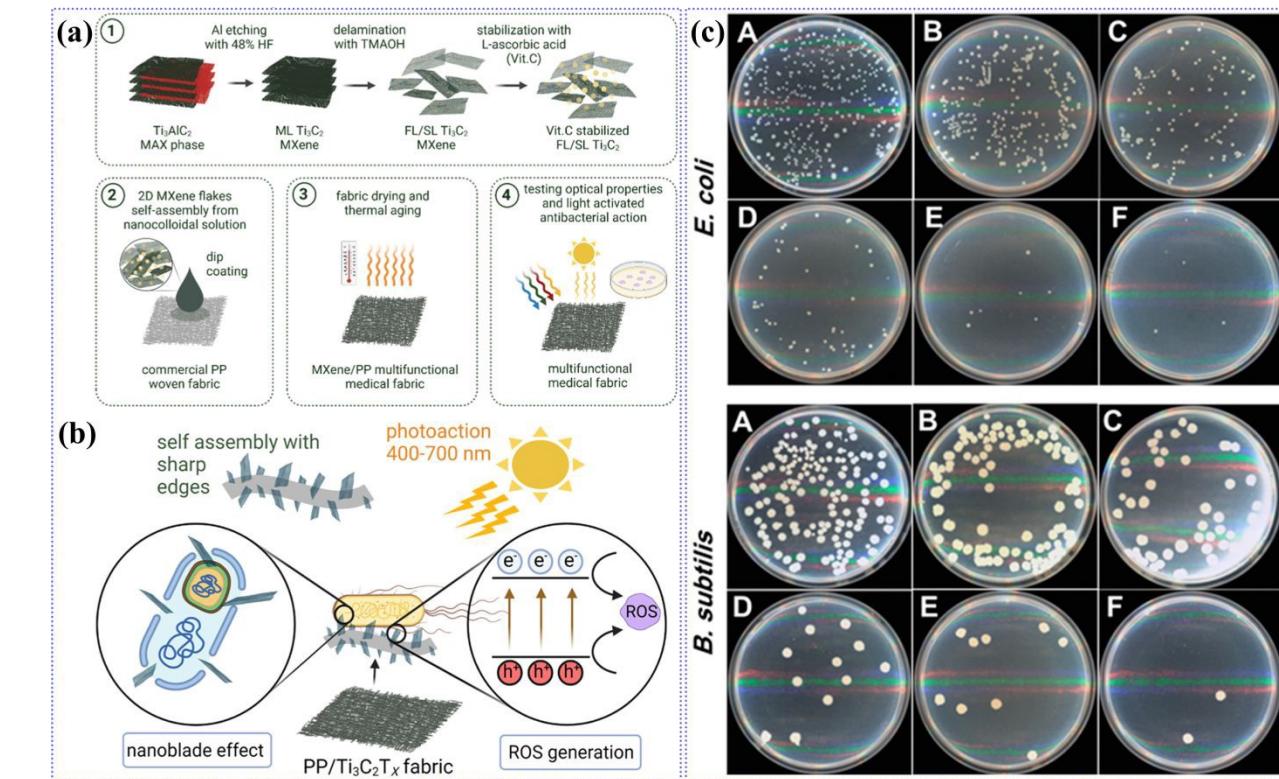
29 A study on the tunable antibacterial activity of a polypropylene (PP) fabric coated with Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub>  
30 MXene flakes, coupling the nano-blade effect with reactive oxygen species (ROS) generation was



1 conducted<sup>75</sup>. In this study, an antibacterial medical fabric using a straightforward self-assembly  
2 process was developed, wherein delaminated  $Ti_3C_2T_x$  MXene flakes were arranged on the surface  
3 of PP fibers (Figure 18a). By varying the amount of MXene in the coating solution from 1 to 32  
4 mg/mL, they achieved edge-on assembly of MXene flakes on the PP surface, allowing the  
5 monitoring of band gap evolution for a restacked structure. Characterization of the PP/ $Ti_3C_2T_x$   
6 nanocomposite revealed highly effective antibacterial properties, a robust coating, and excellent  
7 chemical/thermal stability. In-vitro microbiological studies against both Gram-positive  
8 *Staphylococcus aureus* as well as Gram-negative *Escherichia coli* demonstrated that PP/ $Ti_3C_2T_x$   
9 reduced bacterial viability up to 100%. This effect was attributed to a synergistic combination of  
10 physical contact causing membrane stress and light-induced ROS generation. The antibacterial  
11 mechanism in PP/  $Ti_3C_2T_x$  fabrics involved synergistic membrane stress mediated by the physical  
12 contact of sharp edges (nano-blade effect) of MXene flakes, along with the generation of ROS  
13 (Figure 18b). Before this,  $Ti_3C_2T_x$  MXene exhibited antibacterial properties. Rasool et al.  
14 investigated  $Ti_3C_2T_x$  against *E. coli* and *B. subtilis* using bacterial growth curves and agar plates<sup>74</sup>.  
15  $Ti_3C_2T_x$  showed higher antibacterial efficiency against both *E. coli* and *B. subtilis* compared to  
16 graphene oxide. The concentration-dependent antibacterial activities of  $Ti_3C_2T_x$  in aqueous  
17 suspensions (Figure 18c). The top frame (Right side-top, Figure 18c (A-F)) shows photographs of  
18 agar plates where after a 4-hour treatment, the *E. coli* bacterial cells were subjected to recultivation  
19 with different concentrations of  $Ti_3C_2T_x$ : 0  $\mu\text{g}/\text{mL}$  (A), 10  $\mu\text{g}/\text{mL}$  (B), 20  $\mu\text{g}/\text{mL}$  (C), 50  $\mu\text{g}/\text{mL}$   
20 (D), 100  $\mu\text{g}/\text{mL}$  (E), and 200  $\mu\text{g}/\text{mL}$  (F). The bottom frame (Right side-down, Figure 18c(A-F))  
21 shows photographs of agar plates with *B. subtilis* bacterial cells treated similarly. At a  
22 concentration of 200  $\mu\text{g}/\text{mL}$ ,  $Ti_3C_2T_x$  resulted in over 98% bacterial cell viability loss within 4  
23 hours of exposure, as validated by regrowth curve analysis and colony forming unit (CFU).  
24 Electron microscopic analysis and lactate dehydrogenase (LDH) release assay revealed damage to  
25 the cell membrane, leading to the release of cytoplasmic materials.

26





**Figure 18.** Antibacterial activity of MXene-polymer nanocomposites. (a) Illustration showing a facile approach to obtain  $\text{Ti}_3\text{C}_2\text{T}_x$ -modified PP medical fabrics ( $\text{PP}/\text{Ti}_3\text{C}_2\text{T}_x$  nanocomposites) with exceptional antibacterial properties, adjustable optical characteristics, and impressive thermal and chemical stability. (b) Schematic diagram showcasing the antibacterial activity in  $\text{PP}/\text{Ti}_3\text{C}_2\text{T}_x$  nanocomposites, highlighting the synergistic effect of the physical nano blade action and the generation of reactive oxygen species. Reproduced with permission from ref.<sup>75</sup>. Copyright 2022, American Chemical Society. (c) Concentration-dependent antibacterial activities of  $\text{Ti}_3\text{C}_2\text{T}_x$  in aqueous suspensions. The top frame (Right side-top, Figure A-F) shows photographs of agar plates where after a 4-hour treatment, the *E. coli* bacterial cells were subjected to recultivation with different concentrations of  $\text{Ti}_3\text{C}_2\text{T}_x$ : 0  $\mu\text{g}/\text{mL}$  (A), 10  $\mu\text{g}/\text{mL}$  (B), 20  $\mu\text{g}/\text{mL}$  (C), 50  $\mu\text{g}/\text{mL}$  (D), 100  $\mu\text{g}/\text{mL}$  (E), and 200  $\mu\text{g}/\text{mL}$  (F). The bottom frame (Right side-bottom, Figure A-F) displays photographs of agar plates with *B. subtilis* bacterial cells treated similarly. The study utilized bacterial suspensions in deionized water as a control, without the presence of  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene. Reproduced with permission from ref.<sup>74</sup>. Copyright 2016, American Chemical Society.

MXenes can be utilized for their antibacterial properties, as shown in a study where micrometer-thick  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene membranes were prepared by filtration onto a polyvinylidene fluoride (PVDF) support.<sup>333</sup> To assess their bactericidal effects, the modified  $\text{Ti}_3\text{C}_2\text{T}_x$  membranes were tested against *E. coli* and *B. subtilis* using two methods: bacterial growth on the membrane surface and exposure of the membrane to bacterial suspensions. The results showed that the fresh  $\text{Ti}_3\text{C}_2\text{T}_x$  MXene membranes exhibited an antibacterial rate of over 67% against *E. coli* and 73% against *B. subtilis*, compared to the control PVDF membrane, under the same conditions. Interestingly, the

aged  $Ti_3C_2T_x$  membrane displayed even higher efficacy, with over 99% growth inhibition observed for both bacterial strains.

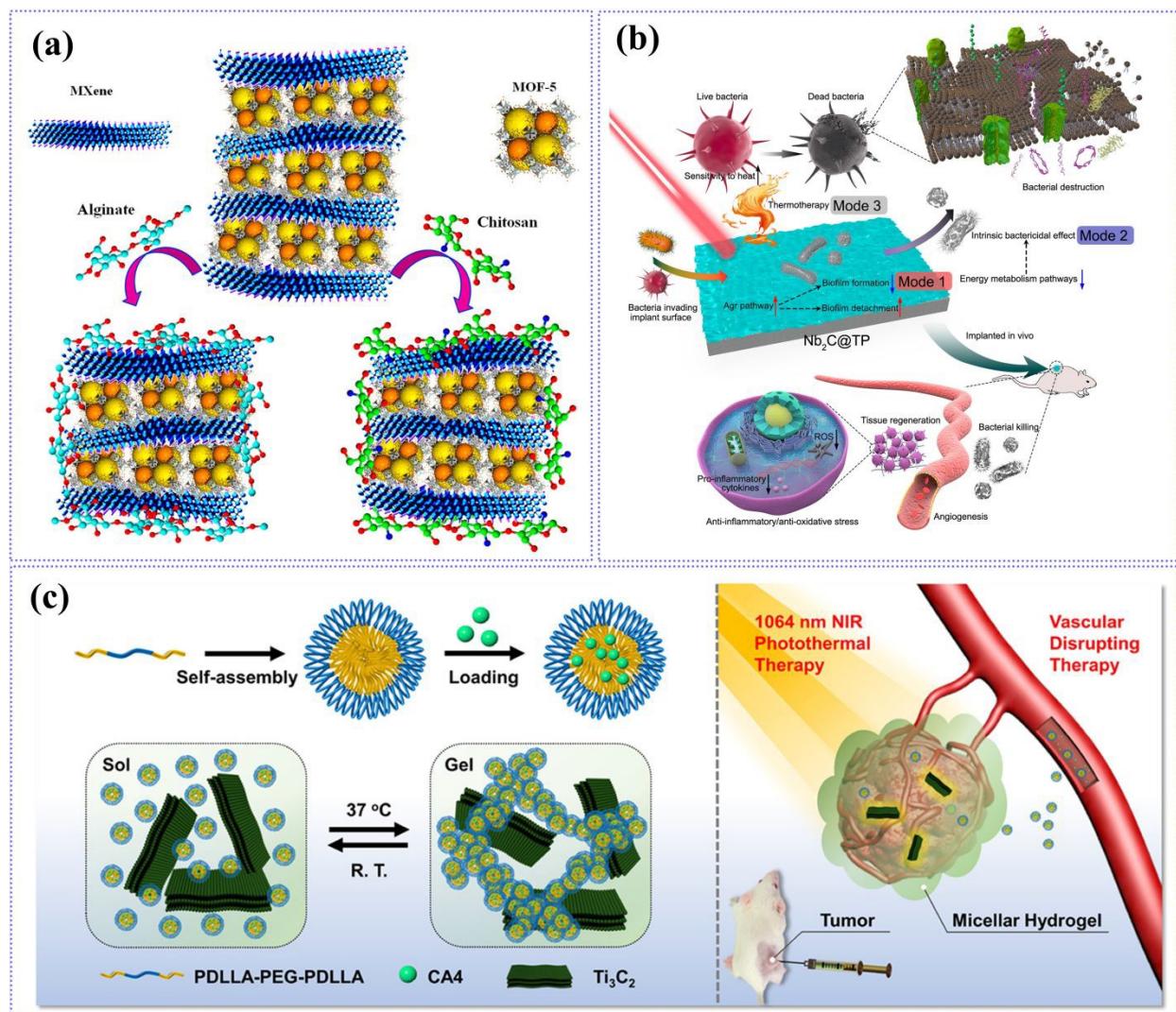
### 7.7.2 Drug delivery and photothermal therapy

MXene-polymer nanocomposites have promising applications in drug delivery, anticancer, antibacterial biofilms, etc.<sup>332, 334</sup> Rabiee et al. developed an innovative nanocarrier using inorganic MXene/MOF-5 (metal-organic frameworks) nanostructures for co-delivery of the drug doxorubicin (DOX) and gene pCRISPR<sup>335</sup>. This study presents a nanocarrier approach for efficient co-delivery of drugs and genes for biomedical applications. To enhance bioavailability and interaction with pCRISPR, the nanomaterial was coated with alginate and chitosan. The polymer-coated nano-systems doxorubicin delivery and cytotoxicity were evaluated on HEK-293, PC<sub>12</sub>, HepG<sub>2</sub>, and HeLa cell lines. The chitosan-coated nanocarriers demonstrated superior cell viability, with over 60% relative cell viability in all tested cell lines. The alginate-coated nanocarriers ranked second, showing more than 50% relative cell viability across all cell lines. The cytotoxicity was dose-dependent, with longer treatment times leading to reduced cell viability. The nanocarriers were modified to become suitable, stimuli-responsive, and equipped with a capping agent. To achieve this, chitosan and alginate were used to modify the nanocarriers (Figure 19a). Polymer solutions of alginate and chitosan were prepared and reacted in the dark for 7 hours. The resulting suspensions were mixed with drug-free (MXene/MOF-5) and drug-loaded (MXene/MOF-5-DOX) nanocarriers for 6 hours at room temperature. After 24 hours on various cell lines, MXene/MOF-5 showed cell viabilities of 38.7%-14.3% at 0.1  $\mu$ g/mL and 27.6%-9.9% at 10  $\mu$ g/mL, with a drug payload efficiency of 35.7%. Chitosan-based nanocarriers achieved a green fluorescent protein (GFP)-positive efficiency of 25.8% in gene delivery studies. Yang et al. developed a clinical implant based on Nb<sub>2</sub>C MXene/titanium plate (Nb<sub>2</sub>C@TP) for bacterial infection removal and for regeneration of tissues<sup>336</sup>. This implant offers practical multimodal anti-infection functions. The Nb<sub>2</sub>C nanosheets (NSs) were decorated onto amidated TPs (TPs-NH<sub>2</sub>) via electrostatic interactions, resulting in the formation of Nb<sub>2</sub>C@TP. The Nb<sub>2</sub>C@TP plays a crucial role in suppressing bacteria through multiple modes (Figure 19b). When bacteria attempt to attack the implant surface, Nb<sub>2</sub>C@TP activates the accessory gene regulator (Agr), which prevents bacterial adherence and promotes biofilm detachment. Nb<sub>2</sub>C@TP directly induces bacterial death by regulating the essential metabolic pathways such as the tricarboxylic acid (TCA) cycle and the



phosphotransferase system (PTS) pathway. These combined mechanisms effectively combat bacterial infection.

Researchers have created a biodegradable nanocomposite micellar hydrogel delivery system with unique functionalities of NIR-II photothermal ablation and vascular disruption, enabling minimally invasive antitumor therapy using  $\text{Ti}_3\text{C}_2\text{T}_x$  and poly(d,l-lactide)-poly(ethylene glycol)-poly(d,l-lactide) (PDLLA-PEG-PDLLA, PLEL) triblock copolymer micelle<sup>337</sup>.  $\text{Ti}_3\text{C}_2$  and CA4 (natural polymer) were selected as the photothermal therapy (PTT) agent and vascular disrupting agent (VDA), respectively, for the development of the nanocomposite micellar hydrogel with dual functionalities in minimally invasive antitumor therapy (Figure 19c).



**Figure 19.** Biomedical applications of MXene polymer nanocomposites in drug delivery and photothermal therapy. (a) Schematic illustration of MXene/MOF-5 and its alginate and chitosan nanostructures. The modification process involves the integration of chitosan and alginate onto the



nanocarriers, resulting in stimuli-responsive properties and the incorporation of a capping agent. Reproduced with permission from ref.<sup>335</sup>. Copyright 2021, American Chemical Society. (b) The trimodal bacterial killing strategy of Nb<sub>2</sub>C@TP. This strategy involves biofilm resistance, intrinsic bactericidal effects, and thermal ablation of bacteria. Additionally, Nb<sub>2</sub>C@TP demonstrates promising in vivo tissue regeneration properties. Reproduced with permission from ref.<sup>336</sup>. Copyright 2021, American Chemical Society. (c) The schematic illustration of injectable PLEL-based micellar hydrogels co-delivered with CA4 and Ti<sub>3</sub>C<sub>2</sub> for synergistic NIR-II photothermal and vascular disrupting therapy. Reproduced with permission from ref.<sup>337</sup>. Copyright 2020, American Chemical Society.

The micellar hydrogel system exhibits an impressive photothermal conversion efficiency (41.4% in the 1064 nm window, utilizing a laser power of 1.0 W cm<sup>-2</sup>). Additionally, hydrogel demonstrates prolonged retention at the tumor site, enabling sustained release of therapeutic agents, thereby facilitating comprehensive and effective treatment.

Additionally, MXenes can also be used to create smart 3D network nanoplatforms by integrating Ti<sub>3</sub>C<sub>2</sub> MXene with cellulose hydrogels showcasing light-induced bimodal photothermal/chemotherapy anticancer activity<sup>327</sup>. When incorporating the anticancer drug doxorubicin hydrochloride (DOX), the cellulose/MXene hydrogels exhibit a remarkable ability to enhance the release rate of DOX, significantly accelerating its delivery. Dai et al. designed composite nanosheets based on Ta<sub>4</sub>C<sub>3</sub> MXene for multiple imaging-guided photothermal tumor ablation. The rational selection of MXene composition and surface functionalization facilitated the achievement of this innovative approach<sup>328</sup>. In the study, a redox reaction was initiated on the surface of Ta<sub>4</sub>C<sub>3</sub> MXene, leading to the in-situ growth of manganese oxide nanoparticles (MnO<sub>x</sub>/Ta<sub>4</sub>C<sub>3</sub>). This growth was facilitated by the reducing properties of the nanosheets. Through careful selection of the MXene composition and additional functionalization, the resulting MnO<sub>x</sub>/Ta<sub>4</sub>C<sub>3</sub>-SP composite nanosheets served as high-performance contrast agents. They enabled simultaneous use in computed tomography (CT) for tantalum-based imaging, tumor microenvironment-responsive T1-weighted magnetic resonance imaging (MRI) using the MnO<sub>x</sub> component, and photoacoustic imaging.

The advantages of MXene-polymer nanocomposites in photothermal therapy enable more efficient, targeted, and controlled treatment of diseases, particularly cancer. The combination of the photothermal properties of MXenes with the tunability, biocompatibility, and targeting capabilities of polymers opens new possibilities for non-invasive, localized, and personalized therapeutic approaches.



## 1    7.8 Water desalination and purification membranes

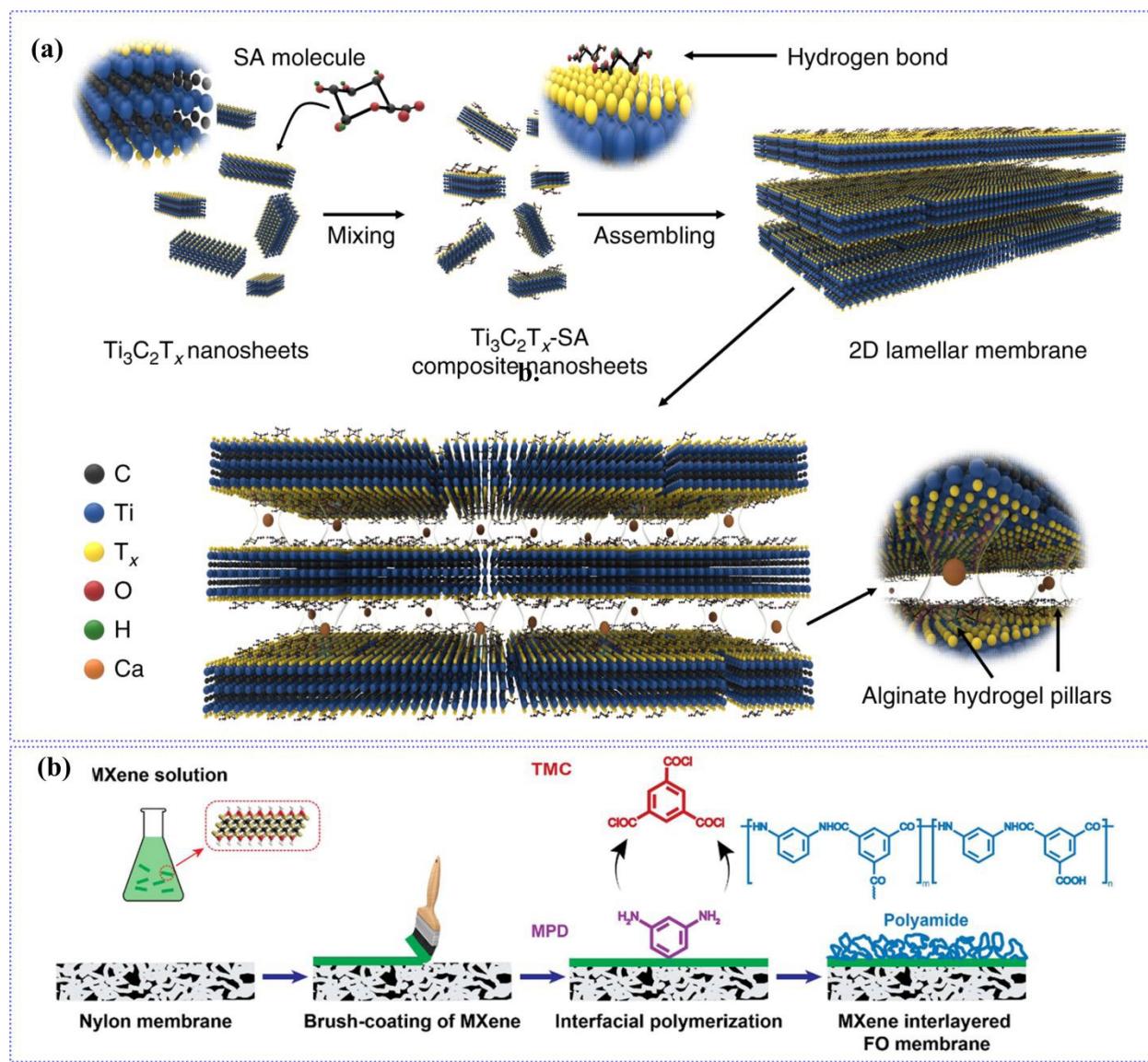
2    MXene-polymer composites offer many advantages in water purification and desalination  
3    applications over MXene<sup>69</sup>. These composites can be easily synthesized, coated onto membranes,  
4    or formed into filters or adsorbents<sup>338</sup>. Polymers can provide a porous and interconnected network  
5    within the composite, increasing the surface area available for adsorption<sup>205, 339</sup>. Numerous studies  
6    have provided evidence that laminar membranes exhibit anomalous transport phenomena, such as  
7    ultrafast and precise ion selectivity, when the d-spacing is comparable to the diameter D of  
8    hydrated ions<sup>340</sup>.

9    MXene-polymer nanocomposites can be utilized to create a super-hydrophilic and underwater  
10   super-oleophobic  $Ti_3C_2T_x$  MXene-based composite membrane. This can be achieved through  
11   vacuum-assisted self-assembly of MXene nanosheets on a porous polyvinylidene fluoride (PVDF)  
12   substrate, followed by in situ mineralization of the photocatalyst  $\beta$ -FeOOH on the membrane  
13   surface<sup>70</sup>. The resulting membrane was treated with HCl and dried under vacuum. The  
14   MXene@CS/TA membrane was prepared by mixing chitosan and tannic acid solutions at pH 3,  
15   immersing MXene in the solution for 12 hours, then rinsing and drying at 30°C under vacuum.  
16   The membrane was subsequently mineralized in FeCl<sub>3</sub> solution, resulting in the MXenes/TA-  
17   FeOOH membrane, which exhibited high permeation flux and superior separation efficiency for  
18   various oil-in-water emulsions.

19   Wang et al. demonstrated a novel approach to stabilize the  $Ti_3C_2T_x$  laminar architecture using  
20   alginate hydrogel pillars<sup>341</sup>. The hybrid SA- $Ti_3C_2T_x$  membrane with a lamellar structure was  
21   prepared by mixing sodium alginate (SA) solution with a diluted  $Ti_3C_2T_x$  colloidal and filtered by  
22   PVDF membrane. Subsequently, the SA- $Ti_3C_2T_x$  membrane was immersed in various multivalent  
23   Mn<sup>+</sup> cross-linking solutions for 4 hours to obtain a cross-linked membrane having hydrogel pillars  
24   in the interlayer spacing (Figure 20a). The flexible membrane was then dried at room temperature  
25   under a vacuum, peeled from the PVDF support, and stored under a vacuum. By pillaring the  
26   membrane with Ca-alginate, the nanochannel diameters ( $7.4 \pm 0.2 \text{ \AA}$ ), resulting in a membrane  
27   that exhibited exceptional permeation cut-off and outstanding sieving properties for different  
28   valent cations. The membrane exhibited a high promise for acid recovery due to its outstanding  
29   H<sup>+</sup>/Fe<sup>2+</sup> selectivity, making it useful for traditional ion exchange membranes. Additionally, an



- 1 ultrathin Mn-alginate pillared membrane with the same d-spacing displayed 100% Na<sub>2</sub>SO<sub>4</sub>  
 2 rejection along with high water permeance.



3   
 4 **Figure 20.** MXene-polymer nanocomposites in water purification/filtration membranes. (a)   
 5 Fabrication process of the sodium alginate (SA) and Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> membrane. Initially, the SA solution   
 6 was mixed with the Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> colloidal solution, leading to firm and homogeneous attachment of   
 7 SA molecules onto the nanosheet surface through hydrogen bonding. Subsequently, the composite   
 8 SA-Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> nanosheets were assembled into a hybrid membrane with a lamellar structure. Finally,   
 9 the SA-Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> membrane was immersed in various multivalent Mn<sup>+</sup> cross-linking solutions   
 10 (Ca<sup>2+</sup>, Ba<sup>2+</sup>, Mn<sup>2+</sup>, and Al<sup>3+</sup>) to obtain the cross-linked membrane with hydrogel pillars in the   
 11 interlayer spacing<sup>341</sup>. (b) Schematic of the fabrication process for MXene/nylon substrates. It   
 12 involves brush-coating MXene onto the surface of commercial nylon membranes, creating a thin   
 13 MXene layer on the nylon substrate. Subsequently, a polyamide membrane is fabricated on top of

1 the MXene/nylon substrate, resulting in the final MXene/nylon/polyamide composite membrane.  
2 Reproduced with permission from ref.<sup>338</sup>. Copyright 2020, American Chemical Society.

3 Additionally, MXene-polymer nanocomposites can be utilized to develop a high-performance  
4 forward osmosis (FO) membrane by interlayering  $Ti_3C_2T_x$  MXene with polyamide<sup>338</sup>. The  
5 fabrication process involved a scalable and straightforward brush-coating of MXene on nylon  
6 substrates, followed by an interfacial polymerization step (Figure 20b). The resulting FO  
7 membrane exhibited high water permeability and low specific salt flux when tested with a sodium  
8 chloride draw solution. It also demonstrated exceptional performance in organic solvent forward  
9 osmosis, showing a significant flux with low specific salt flux using a lithium chloride draw  
10 solution. Additionally, the membrane proved effective for seawater desalination and industrial  
11 textile wastewater treatment applications.

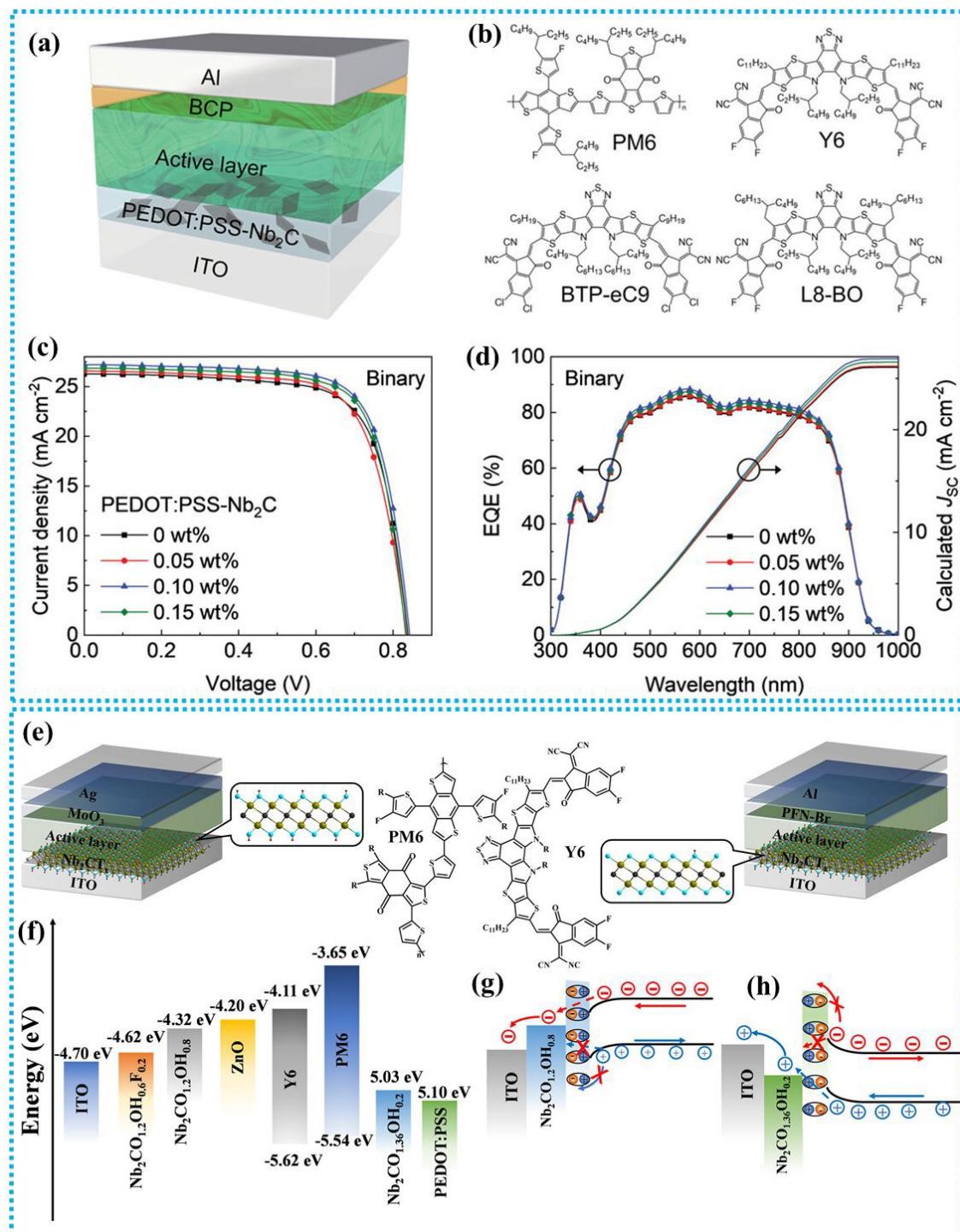
12 All-in-all, the incorporation of polymers into MXene-based materials for water purification and  
13 desalination offers improved adsorption capacity, selectivity, stability, membrane performance,  
14 antifouling properties, scalability, and environmental compatibility<sup>342, 216, 343</sup>. These advantages  
15 make MXene-polymer composites promising candidates for addressing water scarcity, ensuring  
16 clean water supply, and advancing sustainable water treatment technologies.

### 17 **7.9 MXene-polymer nanocomposites for solar cell applications**

18 MXene integrated with polymers can be ideal for solar cell applications due to their ability to  
19 preserve inherent electronic properties and ensure strong interaction with polymer matrices<sup>344</sup>.  
20 This compatibility enhances electrical conductivity, making MXene-polymer composites highly  
21 promising for advancing flexible electronics and photovoltaic devices.  $Nb_2CT_x$  is a significant  
22 member of the MXenes family, which exhibits distinct chemical and physical characteristics as  
23 well<sup>345</sup>. Deng et al. reported a PEDOT: PSS- $Nb_2C$  hybrid hole transport layer (HTL) to improve  
24 the device performance of organic solar cells (OSCs)<sup>346</sup>. They employed PEDOT: PSS- $Nb_2C$   
25 hybrids with varying doping MXene ratios (0.05, 0.10, and 0.15 wt%) by directly mixing the  $Nb_2C$   
26 colloidal aqueous solution with PEDOT: PSS. A 40 nm-thick HTL layer was produced by spin  
27 coating the ITO/glass substrates with PEDOT: PSS aqueous solution or the PEDOT: PSS- $Nb_2C$   
28 hybrid solution for 60 seconds at 3000 rpm followed by deposition of active material, electron  
29 transport layer (ETL), and electrode, respectively. Figure 21a-b presents the schematic layout of  
30 the fabricated device and the chemical structures of the various non-fullerene acceptors (NFAs)  
31 and polymer donor PM6. A higher WF was observed in the case of PEDOT: PSS- $Nb_2C$  hybrid



1 film (5.3 eV), as compared to PEDOT:PSS film (5.0 eV). It is clear that the increased WF better  
 2 fits the WF of PM6 (5.5 eV), which decreases leakage current by suppressing charge  
 3 recombination and facilitating hole extraction<sup>347</sup>. Figure 21c-d shows J-V characteristics and  
 4 external quantum efficiency (EQE) spectra acquired for the OSCs with different Nb<sub>2</sub>C MXene  
 5 ratios in PEDOT:PSS employing the PM6:BTP-eC9 binary active layer.



1 **Figure 21.** MXene-polymer-based solar cells. (a) PEDOT:PSS-Nb<sub>2</sub>C hybrid HTL device  
2 construction. (b) The chemical structure of various NFAs and polymer donor PM6, L8-BO, Y6,  
3 and BTP-eC9. (c) J-V properties and (d) EQE spectra obtained for the solar cells using the  
4 PM6:BTP-eC9 binary active layer with varying Nb<sub>2</sub>C MXene doping ratios in PEDOT:PSS.  
5 Reproduced with permission from ref.<sup>346</sup>. Copyright 2023, Wiley. (e) Diagram of the PSCs device  
6 architecture showing the chemical structure of PM6, Y6, ETL, HTL, and Nb<sub>2</sub>CT<sub>x</sub>. (f) Nb<sub>2</sub>CT<sub>x</sub> is  
7 utilized as the ETL and HTL in the schematic energy level diagram of solar cells. (g) Using  
8 Nb<sub>2</sub>CO<sub>1.2</sub>OH<sub>0.8</sub> as the ETL and (h) Nb<sub>2</sub>CO<sub>1.36</sub>OH<sub>0.2</sub> as the HTL, charge transfer, and extraction in  
9 solar cells. Reproduced with permission from ref.<sup>348</sup>. Copyright 2021, American Chemical Society.

10 Through the use of solution-processable Nb<sub>2</sub>C MXene and by using different NFAs (PM6:Y6,  
11 PM6:BTP-eC9, PM6:BTP-eC9:L8-BO), surface treatments have improved PCE for OSCs based  
12 on binary and ternary systems of active layers. It was proposed that Nb<sub>2</sub>C MXene added to  
13 PEDOT:PSS HTL may efficiently aid in PEDOT and PSS phase separation, enhancing  
14 PEDOT:PSS's conductivity. For OSCs based on the ternary active layer of PM6:BTP-eC9:L8-BO,  
15 the doping ratio of Nb<sub>2</sub>C MXene in PEDOT:PSS was tuned to reach a maximal PCE of 19.33%,  
16 which is currently the highest value among those of single junction OSCs employing 2D materials.  
17 The hybrid HTL improves performance by reducing interface recombination, enhancing hole  
18 mobility, and boosting charge extraction efficiency.

19 A similar study by Huang et al. reported the use of Nb<sub>2</sub>CT<sub>x</sub> that investigated the use of additional  
20 MXenes in the photovoltaic area by treating Nb<sub>2</sub>CT<sub>x</sub> with alkali and annealing treatments to  
21 modify its WF by controlling the surface functional groups<sup>348</sup>. Following a KOH treatment, −F in  
22 pure Nb<sub>2</sub>CT<sub>x</sub> may be substituted with −OH, and lowered the WF from 4.62 (Nb<sub>2</sub>CO<sub>1.2</sub>OH<sub>0.6</sub>F<sub>0.2</sub>)  
23 to 4.32 eV (Nb<sub>2</sub>CO<sub>1.2</sub>OH<sub>0.8</sub>). WF increased to 5.03 eV (Nb<sub>2</sub>CO<sub>1.36</sub>OH<sub>0.2</sub>) as a result of the removal  
24 of one part of the −OH and the transformation of another portion into −O groups upon annealing  
25 at 500 °C. Additionally, this is the first time that these Nb<sub>2</sub>CT<sub>x</sub> groups have been used as the ETL  
26 and PM6:Y6-based polymer solar cells (PSCs) HTL, which has a stellar PCE of 15.22% (ETL)  
27 and 15.03% (HTL). These Nb<sub>2</sub>CT<sub>x</sub> are applied to the PSCs based on PM6:Y6 as a buffer layer,  
28 where Nb<sub>2</sub>CT<sub>x</sub> with KOH treatment is used as ETL, and Nb<sub>2</sub>CT<sub>x</sub> with annealing treatment is used  
29 as HTL. Figure 21e shows the schematic of the PSCs structures with tuned Nb<sub>2</sub>CT<sub>x</sub>  
30 (Nb<sub>2</sub>CO<sub>1.2</sub>OH<sub>0.8</sub>, Nb<sub>2</sub>CO<sub>1.36</sub>OH<sub>0.2</sub>) used as the ETL and HTL. Figure 21f shows the energy level  
31 diagram with Nb<sub>2</sub>CT<sub>x</sub> used as the ETL and HTL. From this, it can be seen that the Nb<sub>2</sub>CO<sub>1.2</sub>OH<sub>0.8</sub>  
32 (or Nb<sub>2</sub>CO<sub>1.36</sub>OH<sub>0.2</sub>) exhibits a well-matched energy level compared to Nb<sub>2</sub>CO<sub>1.2</sub>OH<sub>0.6</sub>F<sub>0.2</sub> in PSCs,  
33 which reduces the electron (or hole) barrier height. Moreover, for Nb<sub>2</sub>CO<sub>1.2</sub>OH<sub>0.8</sub>, the dipolar



1 interlayer induced by  $-\text{OH}$  will form an electric field pointing from the active layer toward  
2  $\text{Nb}_2\text{CT}_x$ , which will facilitate the transport of the electrons but block the transport of the holes  
3 (Figure 21g). On the other hand, with  $\text{Nb}_2\text{CO}_{1.36}\text{OH}_{0.2}$ , the dipolar interlayer created by  $-\text{O}$  will  
4 provide an electric field that points from  $\text{Nb}_2\text{CT}_x$  in the direction of the active layer, facilitating  
5 the movement of the holes but preventing the motion of electrons (Figure 21h).

6  $\text{V}_2\text{C}$  MXene has also demonstrated great potential for solar cell applications due to its exceptional  
7 electrical properties, superior mechanical qualities, and high transmittance<sup>73</sup>.  $\text{V}_2\text{C}$  MXene exhibits  
8 excellent hydrophilicity, adjustable work function, strong electrical conductivity, and better  
9 transparency. Gu et al. improved the properties of organic solar cells by placing a layer of  $\text{V}_2\text{C}$   
10 material between ITO and PEDOT: PSS significantly improved the performance of PM6:BTP-  
11 eC9-based devices<sup>73</sup>. Using a 2D nanosheet material  $\text{V}_2\text{C}$  in combination with PEDOT: PSS, a  
12 high-performance  $\text{V}_2\text{C}/\text{PEDOT}: \text{PSS}$  composited HTL was created, offering superior  
13 transmittance and strong electrical conductivity. In addition, the  $\text{V}_2\text{C}/\text{PEDOT}: \text{PSS}$  composite  
14 HTL outperformed the pure PEDOT: PSS interface layer in terms of device performance and  
15 photovoltaic properties. In comparison to the 17.41% efficiency of the pure PEDOT: PSS interface  
16 device, the  $\text{V}_2\text{C}/\text{PEDOT}: \text{PSS}$ -based composite interface device exhibited a notable rise to 18.17%.  
17 According to the carrier dynamics study, the addition of the  $\text{V}_2\text{C}$  layer increased the number of  
18 charge-transfer paths with PEDOT: PSS, which enhanced charge transfer and collection and even  
19 reduced the performance of charge combinations. The findings showed that adding 2D material  
20  $\text{V}_2\text{C}$ , which has excellent conductivity and permeability, offers an efficient way to improve the  
21 performance of solar cells.

## 22     **8. Limitations of MXenes in Polymer Nanocomposites for Various Applications**

23 There is no doubt that MXenes when added in polymers can improve the overall properties of the  
24 resulting nanocomposites. However, their practical implementation across diverse applications is  
25 hindered by inherent limitations such as MXene oxidation susceptibility, brittleness of polymer at  
26 higher MXene concentrations, color change due to MXene, and poor dispersion of MXenes in  
27 many solvents. These challenges are particularly critical when MXenes are combined with  
28 polymers for specific applications, where uniform distribution and long-term stability are essential.  
29 The limitations of MXenes in polymer nanocomposites for various applications are as follows:



- 1     1. **Energy Storage:** Oxidation degradation in MXenes affects their conductivity and  
2     electrochemical characteristics, reducing the overall energy storage performance. Higher  
3     MXene concentration may lead to brittleness of nanocomposite which can limit mechanical  
4     flexibility, impacting stability during cyclic stability studies. Poor dispersion in polymers  
5     may also result in non-uniform coatings, lowering the specific capacitance and energy  
6     density.
- 7     2. **Sensors:** Oxidation of MXenes can reduce sensitivity and selectivity due to reduced  
8     conductivity. Beyond optimized MXene concentrations impact the mechanical durability  
9     of sensors which can limit their flexibility. Poor dispersion results in polymers may result  
10    in non-uniform sensing layers, affecting the reliability and repeatability of sensors.
- 11    3. **3D/4D Printing:** The brittleness of MXene-polymer composites restricts their flexibility  
12    and printability, posing challenges for fabricating complex structures. MXenes oxidation  
13    during post-processing can further compromise the mechanical strength and structural  
14    stability of these nanocomposites. Poor dispersion of MXenes within polymer matrices  
15    impairs resolution and uniformity, which can limit the controlled precision and  
16    performance of printed architectures.
- 17    4. **EMI Shielding:** When MXenes are incorporated into polymers, oxidation-induced  
18    degradation, mechanical brittleness, and poor dispersion can negatively impact EMI  
19    shielding performance. Oxidation at the MXene-polymer interface can reduce  
20    conductivity, lowering shielding effectiveness. Despite polymer flexibility, MXenes may  
21    still contribute to brittleness, weakening the composite under stress. Poor dispersion of  
22    MXenes leads to uneven conductivity, resulting in inhomogeneous shielding layers and  
23    reduced EMI performance. Proper dispersion and oxidation control are crucial for  
24    maximizing the effectiveness of polymer-MXene composites in EMI shielding  
25    applications.
- 26    5. **Anti-Corrosion Applications:** In anti-corrosion applications, oxidized MXenes can  
27    degrade their protective barriers, reducing efficiency. Poor dispersion of MXenes can cause  
28    uneven coatings, leading to defects and corrosion pathways. High concentrations of  
29    MXenes can lead to fragility that can result in cracks, compromising the protective  
30    performance. Effective dispersion and oxidation control are crucial for maintaining the  
31    integrity of MXene-based coatings.



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- 1     6. **Flexible Electronics:** In MXene-polymer composites for flexible electronics, the
  - 2         overconcentration of MXenes in polymers may lead to brittleness of MXenes which limits
  - 3         flexibility, affecting stretchability and durability. Oxidation-induced color changes alter
  - 4         optical properties, restricting their use in transparent or visual devices. Poor dispersion of
  - 5         MXenes within the polymer matrix leads to reduced conductivity and structural
  - 6         inconsistencies, which degrade performance. Effective dispersion and oxidation control are
  - 7         crucial for enhancing the properties of MXene-based polymer composites in flexible
  - 8         electronic applications.
  - 9     7. **Antimicrobial Applications:** When MXenes are mixed with polymers for antimicrobial
  - 10        applications, their susceptibility to oxidation degradation may reduce antibacterial efficacy
  - 11        over time. Poor dispersion in the polymer matrix leads to uneven distribution,
  - 12        compromising the uniformity of the antimicrobial effect. Proper dispersion and oxidation
  - 13        control are crucial to maintaining the long-term effectiveness of MXene-polymer-based
  - 14        antimicrobial composites.
  - 15     8. **Drug Delivery and Photothermal Therapy:** When MXenes are added to polymers for
  - 16        drug delivery and photothermal therapy, their oxidation sensitivity reduces photothermal
  - 17        efficiency and chemical stability, affecting target delivery precision. Limited
  - 18        biocompatibility requires surface modifications, which may alter the structural integrity of
  - 19        MXenes. Dispersion challenges of MXenes in the polymer matrix hinder uniform drug
  - 20        loading and controlled release, impacting therapeutic effectiveness. Proper surface
  - 21        modification and dispersion control are essential to optimize the performance of MXene-
  - 22        based drug delivery and photothermal therapy systems.
  - 23     9. **Water Desalination and Purification Membranes:** When MXenes are added to polymers
  - 24        for water desalination and purification membranes, MXene oxidation can impact ion
  - 25        selectivity and permeation performance, limiting their reliability and durability. The higher
  - 26        concentration of MXenes may lead to brittleness of the membranes under operational
  - 27        conditions. Limited solvent compatibility results in poor dispersion within the polymer
  - 28        matrix, reducing uniform pore formation and compromising membrane performance.
  - 29        Effective dispersion, oxidation control, and solvent compatibility are crucial for enhancing
  - 30        the long-term performance of MXene-based water desalination and purification
  - 31        membranes.

1       10. **Solar cells:** MXene oxidation lowers conductivity and stability, affecting solar cell  
2       efficiency. High concentrations cause agglomeration, disrupting charge transport, while  
3       poor solvent compatibility results in non-uniform films, compromising light absorption and  
4       carrier mobility. Enhanced dispersion, oxidation resistance, and solvent compatibility are  
5       crucial for improving solar cell performance.

6       **9. Challenges and opportunities in MXene-polymer nanocomposites**

7       **9.1 Challenges**

8       Synthesis of MXene-polymer nanocomposites poses several challenges, which can impact the final  
9       properties and performance of the materials.

10      1. Uniform dispersion of MXenes in polymer matrix: As MXenes tend to agglomerate due to  
11       their high surface energy, ultimately, it can lead to poor interfacial interactions and reduced  
12       mechanical properties of the nanocomposite

13      2. Stability: Dispersion stability is another issue that needs to be addressed. MXene-polymer  
14       nanocomposites can be sensitive to environmental factors as MXenes are prone to oxidation,  
15       leading to potential degradation or loss of functionality over time.

16      3. Interface compatibility: Achieving strong interactions and uniform dispersion of MXene  
17       nanosheets within polymer matrices is crucial for optimizing the properties of nanocomposites.  
18       Surface functionalization for proper interaction is itself a challenging task.

19      4. Scalability and reproducibility: Large-scale synthesis of MXene-polymers nanocomposites  
20       with consistent properties remains challenging, hindering widespread commercial  
21       applications. Processing techniques selection for uniform MXenes dispersion necessary for  
22       high-quality nanocomposites. High-cost instruments may be required for large-scale mixing.

23      5. Mechanical properties: Optimizing the ratio of MXenes and polymers is crucial for any  
24       property. MXene-polymer nanocomposites may face limitations in achieving high mechanical  
25       strength and toughness, especially in certain applications that demand robust materials if  
26       optimization is not suitable for that application.

27      **9.2 Opportunities**

28       Once perfect compatibility between MXenes and polymers is achieved, the MXene-polymer  
29       nanocomposites may offer enhanced mechanical, thermal, electrical, and optical properties in  
30       versatile materials, making them compatible with diverse applications.



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- 1    1. Multifunctionality: The unique properties of MXene-polymer hybrids open up opportunities
  - 2       for developing new nanocomposites with multiple functionalities, enabling versatile
  - 3       applications.
  - 4    2. Biomedical applications: MXene-polymer hybrids, due to their biocompatibility and
  - 5       antibacterial properties, hold promise in drug delivery systems, tissue engineering, and medical
  - 6       implants.
  - 7    3. Energy-related applications: MXene-polymer nanocomposites, due to their porous structures,
  - 8       can be employed in energy storage devices to enhance performance and stability.
  - 9    4. Environmental applications: MXene-based nanocomposites have potential in environmental
  - 10      remediation, sensing, and water purification membranes owing to their better adsorption and
  - 11      catalytic traits.
  - 12    5. New-age technology integration: The combination of cutting-edge technologies, such as
  - 13       nanocomposite fabrication, the Internet of Things (IoT), and artificial intelligence (AI), holds
  - 14       tremendous potential in designing and developing future smart materials with enhanced
  - 15       properties and functionalities.
  - 16    6. Hence, MXene-polymer nanocomposites offer exciting prospects for addressing various
  - 17       challenges and capitalizing on their unique properties to explore novel applications in diverse
  - 18       industries. However, further research is needed to overcome existing limitations and fully
  - 19       unlock their potential for practical utilization.

## 20    **10. Future perspectives**

21    The future of MXene-polymer nanocomposites is exceptionally promising, with vast potential

22       across multiple domains. MXenes offer numerous beneficial properties, but these advantages are

23       contingent on preventing oxidation. By addressing this challenge, the full spectrum of MXene's

24       capabilities can be harnessed by integrating these with polymers, paving the way for

25       groundbreaking applications and advancements in various fields. Ongoing advancements in

26       MXene synthesis, functionalization, and nanocomposite fabrication are likely to yield innovative

27       materials with enhanced properties such as lightweight structures, improved mechanical strength,

28       superior electrical conductivity, and increased thermal stability. These developments could

29       revolutionize industries from aerospace to electronics. Additionally, MXene-based

30       nanocomposites show great promise in sustainable technologies, potentially leading to more

31       efficient and eco-friendly solutions in energy storage, water purification, and environmental

1 remediation. In the biomedical field, the biocompatibility and antibacterial properties of MXene-  
2 polymers hold potential for breakthroughs in drug delivery systems, tissue engineering scaffolds,  
3 and bioactive coatings for implants. The tunable properties of these nanocomposites also pave the  
4 way for the creation of smart materials capable of responding to external stimuli, which could  
5 transform applications in sensors, actuators, and adaptive coatings. Moreover, the integration of  
6 multiple functionalities within a single MXene-polymer material opens exciting possibilities for  
7 multifunctional devices that perform various tasks simultaneously. Combining MXene-polymers  
8 with other nanomaterials, such as graphene, metal nanoparticles, or quantum dots, may lead to new  
9 synergistic effects and advanced functionalities. Furthermore, the intersection of nanocomposite  
10 fabrication technologies with artificial intelligence and the Internet of Things promises to enhance  
11 the design and deployment of advanced smart materials. As research and interdisciplinary  
12 collaboration continue, MXene-polymer nanocomposites are set to address global challenges and  
13 drive significant innovations across a range of industries.

## 14 **11. Conclusions**

15 In conclusion, this comprehensive review emphasizes the synthesis methods and diverse  
16 applications of MXene-polymer nanocomposites while keeping in mind the serious issue of  
17 MXene oxidation. The various fabrication techniques, such as solution blending, in-situ  
18 polymerization, LBL assembly, and electrospinning, offer opportunities to tailor the properties of  
19 these nanocomposites for specific applications. MXenes can be easily hybridized with various  
20 polymers such as PVA, PDMS, PPy, PEDOT:PSS, polyaniline, polypropylene, polyurethane, and  
21 many biopolymers. MXene-polymer nanocomposites exhibit conductivity, stability, flexibility,  
22 biocompatibility, and ion diffusion, leading to enhanced performance and durability in various  
23 devices. The incorporation of polymers in MXene-based sensors enhances sensitivity, selectivity,  
24 flexibility, and response time, enabling more accurate and efficient detection of target analytes.  
25 MXene-polymer composites provide EMI shielding effectiveness, lightweight, and flexible  
26 characteristics, making them suitable for applications in the electronics, telecommunications, and  
27 aerospace industries. The combination of MXenes with polymers offers flexibility, stretchability,  
28 and improved mechanical properties, enabling the development of flexible electronic devices.  
29 MXene-polymer composites inculcate higher porosity in the nanocomposite which can increase  
30 the charge storage capacity. MXene-polymer composites offer enhanced photothermal conversion  
31 efficiency, controlled drug delivery, enabling effective cancer treatment, and wound healing.



1 MXene-polymer composites provide enhanced adsorption capacity, selective adsorption,  
2 improved stability, membrane performance, antifouling properties, scalability, and environmental  
3 compatibility, making them effective materials for water purification and desalination processes.  
4 These advantages highlight the potential of MXene-polymer composites in addressing various  
5 challenges and advancing technological applications. The unique properties and synergistic effects  
6 resulting from the combination of MXenes and polymers create exciting opportunities in various  
7 fields, enabling the development of efficient, sustainable, and functional materials and devices.  
8 This advancement ensures that MXene oxidation will not hinder the progress toward innovative  
9 solutions.

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12 **Author contributions:**

13 Sunil Kumar – original draft, conceptualization, and data curation; Syed Muhammad Zain Mehdi  
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15 Kumar – review and editing; Amit Aherwar – review and editing; Sudhanshu Singh – review and  
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17 **Conflict of Interests**

18 The authors declare that there is no conflict of interest.

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27





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1



2

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## Declaration of generative AI and AI-assisted technologies in the writing process

During the preparation of this work, the author(s) used ChatGpt to improve the grammar. After using this tool/service, the author(s) reviewed and edited the content as needed and take(s) full responsibility for the content of the publication.

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**Data Availability Statement:**

No new data was created in this review. All data referenced are from previously published sources and are available in the respective cited articles.

