

1 **Two Dimensional MXenes as Emerging Paradigm for Adsorptive Removal of**
2 **Toxic Metallic Pollutants from wastewater**

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18 **Abstract**

19 Effective methods for removing harmful metals from wastewater have had a huge impact on
20 reducing freshwater scarcity. Because of its excellent removal effectiveness, simplicity and low
21 cost at ambient conditions, adsorption is one of the most promising purifying approaches. MXene-
22 based nanoarchitectures have proven to be effective adsorbents in a variety of harmful metal
23 removal applications. This owes from the distinctive features such as, hydrophilicity, high surface

24 area, electron-richness, great adsorption capacity, and activated metallic hydroxide sites of
25 MXenes. Given the rapid advancement in the design and synthesis of MXene nanoarchitectures for
26 water treatment, prompt updates on this research area are needed that focus on removal of toxic
27 metal, such as production routes and characterization techniques for the advantages, merits and
28 limitations of MXenes for toxic metal adsorption. This is in addition to the fundamentals and the
29 adsorption mechanism tailored by the shape and composition of MXene based on some
30 representative paradigms. Finally, the limits of MXenes are highlighted, as well as their potential
31 future research directions for wastewater treatment. This manuscript may initiate researchers to
32 improve unique MXene-based nanostructures with distinct compositions, shapes, and
33 physiochemical merits for effective removal of toxic metals from wastewater.

34 **Keywords:** 2D-MXenes; MXene nanocomposite; wastewater; Adsorption; Toxic metal Pollutants

35 **1. Introduction**

36 As fast industrialization continues, various toxins have been released into water without being
37 properly cleaned, causing serious environmental contamination and danger to human health
38 (Jasper et al., 2017). Generally, Organic and inorganic pollutants are the two types of contaminants
39 that can be found in the environment. Typical dye compounds such as methylene blue, which are
40 released by manufacturers making paper, paint, textiles, and other products, are among the organic
41 pollutants (Karaçetin et al., 2014). While heavy metal ions (HMIs) and radionuclide are among the
42 inorganic pollutants in wastewater (Ahmad and Mirza, 2018; Mirza and Ahmad, 2018; Zhang et
43 al., 2018). Because of their carcinogenicity and toxicity, they have adverse impact on natural
44 environment and living organisms in general. Some of the maximum allowable contaminant level
45 of heavy metals are as follows, Arsenic: .05 mg/l, Cadmium: .005 mg/l Lead: .015 mg/l, Mercury:
46 .002 mg/l, Chromium: .1, Selenium: .05 mg/l, Antimony: .006 mg/l. Because some of them can

47 bioaccumulate, the harm they cause to living organisms may be greater than that caused by
48 pollutants that cannot bioaccumulate (Berrios et al., 2012; Karaçetin et al., 2014). As a result, one
49 of the most important predictors of long-term industrial prosperity has been the deployment of
50 effective treatment procedures for the elimination of harmful toxins.

51 Adsorption is one of the most extensively employed technique for the purpose due to its appealing
52 properties such as simplicity, cost-effectiveness, and applicability (Ahmad and Mirza, 2018;
53 Burakov et al., 2018; Mirza and Ahmad, 2018; Wu et al., 2019; Mittal et al., 2021). Furthermore,
54 using adsorbent to remove toxicants minimizes the production of secondary pollutants because the
55 adsorbents absorb rather than reacting with the contaminants (Wu et al., 2019). A number of
56 documented reports are present in the literature, which discuss the utility of powdered or granular
57 activated carbon, chitosan, and kaolin etc. are the few among many to be used as adsorbents for
58 the purpose (Oguz and Keskinler, 2005; Wang et al., 2010; Zhu et al., 2010). The greater surface
59 area and high porosity of these materials makes them an ideal candidate for the environmental
60 remediation. Recently, an emerging class of nanomaterials such as two-dimensional (2D) have
61 extensively been exploited for the efficient removal of a variety of environmental contaminants.
62 The distinctive features of these 2D nanomaterials warrant their applicability in adsorptive removal
63 (Fu et al., 2018; Wu et al., 2019). The use of nanomaterial-based adsorbents for the treatment of
64 organic and inorganic contaminants in water has increased due to the unique features of 2D
65 nanomaterials, i.e. carbon-based nanomaterials (Atkovska et al., 2018). Nanomaterial-based
66 adsorbents frequently have thin structures, large specific surface areas, and plentiful functional
67 sites, as compared to the huge and bulkier construction of traditional adsorbents (Zhang et al.,
68 2018). Because adsorbents must have a high level of contact with adsorbates and a sufficient
69 surface area to function well, hence the nanomaterials are thought to have the ability to address

70 both inorganic and organic adsorbates (Yang et al., 2019). MXene, a new class of 2D nanomaterials
71 derived from a family of transition metal nitride or carbide compounds, has recently piqued interest
72 in a variety of fields.

73 Owing to their excellent properties such as greater surface area, eco-friendly, greater chemical
74 stability, hydrophilicity, and electrical/thermal conductivity, MXenes are ideal materials for a
75 variety of applications, such as hydrogen storage (Hu et al., 2013), lithium-ion battery (Naguib et
76 al., 2012), supercapacitor (Zhu et al., 2016), semiconductor (Gao et al., 2016), and environmental
77 applications (Ciou et al., 2019). Particularly, the probable environmental applications comprise of
78 membrane filtration, photocatalysis and adsorption to eradicate contaminants, via MXenes and
79 MXene-based composite materials as adsorbents for the elimination of inorganic and organic
80 pollutants from water have extensively been studied (Rasool et al., 2017).

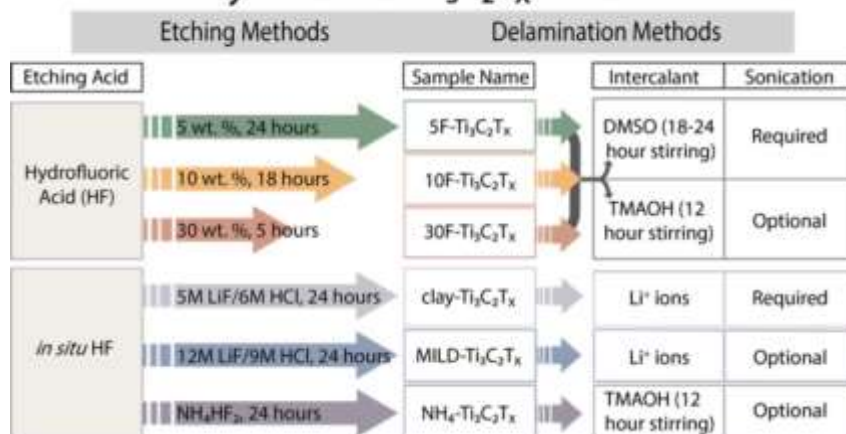
81 Herein, the main purpose of the study is to comprehend the overall knowledge of MXenes and
82 their composites as potential adsorbent for the removal of inorganic impurities such as heavy metal
83 ions and radionuclides from water. In order to achieve the goal, this study will focus on the key
84 aspects of manipulating the composition and shape of MXenes and MXene based nanocomposites
85 for the removal of toxic metal from wastewater, such as manufacturing strategies and
86 characterization methodologies, as well as their formation mechanisms. The limitations and
87 advantages of these materials as adsorbents of toxic heavy metals and radionuclides are reviewed,
88 along with their adsorption mechanism, supported by several descriptive paradigms. Then,
89 perspectives and outlooks for future research in the field of removing these analytes (heavy metal
90 ions and radionuclides) are suggested.

91 **2. Characterization of MXenes and Their Preparation**

92 MXenes, a potentially new class of two dimensional (2D) materials, have been the subject of a
93 number of recent book chapters and review papers that have discussed their distinctive features,
94 potential applications, and syntheses (Ng et al., 2017; Zhang et al., 2018; Habib et al., 2019;
95 Melchior et al., 2019). As a result, the focus of this review is solely on the adsorption behavior and
96 characterization of certain MXene structures in wastewater treatment, with an emphasis on particle
97 entrapment methods and the significance of unique surface functionalization in operational
98 efficiency. The term “MXenes” represents a class of nanoparticles, sharing the general formula
99 based representation as $M_{n+1}X_nT_x$ ($n = 1-3$). In this formula M stands for transition metals such
100 as, Mo, Nb, Sc, Hf, Cr, Ti, Ta, Zr, V, etc. while X is a carbon or nitrogen atom and T_x is the
101 variable surface termination which is highly dependent on the manufacturing method and
102 requirement of properties of the formed MXene. These terminals may include fluorine, oxygen or
103 hydroxyl moieties but not limited to them. The development in the field of MXenes as 2D materials
104 using different methods and raw materials is becoming increasingly popular which is also
105 emerging a new three dimensional (3D) constructs/architectures (Ng et al., 2017; Xiu et al., 2018).
106 The layered architecture of M ($n + 1$) and X (n) layers respectively, which are termed 3D pores
107 inside their nanoscale configuration, is what brands MXenes so intriguing (Anasori and Gogotsi,
108 2019). While the majority of MXenes are made up of just one transition metal, some varieties exist
109 in which more than one metal is involved, either in a layered fashion, random distribution or in
110 well-ordered pattern. Generally, the selective etching by A group elements using their MAX phase
111 is applied for the fabrication of MXenes. The layered nitrides and carbides (X-elements) represents
112 the MAX phase in MXenes structure which are sandwich between A layers of group III A/IVA
113 such as Si or Al (not limited to them may also include Pb, P, As, S, Ga, Sn, Ge, In, Cd, and Tl)
114 and M layers of transition metals (Anasori and Gogotsi, 2019). Among the most commonly

115 commercially available MAX phase employed is Ti_3AlC_2 . As a result, the majority of MXenes
116 research focuses on those with the formula $Ti_3C_2T_x$, where T stands for surface terminations like
117 $-OH$, F^- , or $-O$. The selective chemical etching methodology is being employed for the fabrication
118 of $Ti_3C_2T_x$. The hydrofluoric acid (HF) is used as an etching agent, accompanied by the use of
119 dimethyl sulfoxide as delaminating agent under sonication. Moreover, to create fluoride free
120 surface termination the dry etching technique is widely exploited in comparison to wet etching.
121 This can increase the suitability of activating the MXenes surface and its applicability in a broader
122 context. The stacking of MXene layers and effects of various delamination and etching procedures
123 on generated MXene formulae are portrayed in Figure 1 (Alhabeab et al., 2017). Herein, the
124 influence of various preparatory methods of MXene and their structure, morphologies, and surface
125 terminations are examined in relation to the hazardous metal. Before going into depth about
126 MXenes' ability to remove harmful metal particles, it's important to note that one of the most
127 significant roadblocks to MXenes' commercialization is its thermodynamically metastable
128 condition. The remarkable high surface energy of MXenes, especially makes them highly
129 susceptible to degradation. MXene solutions, in particular, oxidize over time, creating TiO_2
130 crystals at the boundaries of MXene flakes and eventually transforming the entire structure into
131 carbon sheets and TiO_2 . The difference between the oxidized and pristine MXene can be clearly
132 marked by discerning the difference in color, as the oxidized solution colored as cloudy white or
133 gray while the pristine MXenes are greenish black in color to the naked eye.

Synthesis of $Ti_3C_2T_x$ MXene



134
 135 **Figure 1.** Preparation of $Ti_3C_2T_x$ using different synthesis routes (direct HF and in situ HF).
 136 Reproduced with permission from (Alhabeab et al., 2017). Copyright 2017 ACS.

137 Generally, the MXenes powder are robust and stable in an oxygen rich atmosphere below 200 °C
 138 (Zhang et al., 2017). For the remediation of toxicant such as metals, TiO_2 is an effective adsorbent
 139 for a variety of analytes including chromium (Almeida et al., 2019), mercury (Ghasemi et al.,
 140 2012) and copper (Cheng et al., 2019). Consequently, a number of MXene based materials are
 141 purposely venerable in hydrothermal environments to attain TiO_2 as surface elements. Multiple
 142 stabilizing strategies for MXene flakes have been investigated, including the use of carbon nano-
 143 plates. This results in the creation of new MXene hybrids reinforced with MoS_2 and carbon
 144 accompanied by the high energy mechanical milling in DMSO demonstrating that the addition of
 145 fluorine to their surfaces can achieve high stability (Wang et al., 2016; Wu et al., 2017).
 146 Prospectively, MXene based compounds with greater shelf lives and higher stability are predicted
 147 to be used in management of wastewater applications by taking fact that the MXene flakes are
 148 exposed to aquatic environment. The fast degradability and fragility of MXenes should be
 149 accountable when designing the systems for the remediation of targeted toxic metal. The profligate
 150 conversion of MXenes into environment friendlier components is advantageous, which may

151 facilitate the operational simplicity in handling the resultant slurry to be used in wastewater
152 management. Further investigations are needed to be carried out in defining their ranges of
153 operation and final efficiency, more research into the applications of MXenes in water treatment,
154 as well as their breakdown after binding with harmful metals or other harmful wastes, is required.

155 **3. Methods and factors effecting for the Removal of Toxic Metal from Wastewater**

156 Over the last few decades, various wastewater management systems have been developed
157 (Burkhard et al., 2000). Among them, reverse osmosis, precipitation, adsorption ion exchange,
158 membrane filtering, and electro-kinetic techniques are all traditional methodologies used for the
159 removal of harmful metal (Vardhan et al., 2019). Even though some of these approaches, such as
160 adsorption and ion exchange, are often employed concurrently, majority of them are used in
161 tandem to isolate the harmful metal and other particles using isolation chambers or reverse
162 osmosis. As a result, the poisonous metal solutes are subsequently converted to solid compounds
163 using adsorption, precipitation, electro-kinetics, a chelating agent or coagulation, and subsequently
164 filtered using different membranes or other collecting methods. Further, the preprocessing stages
165 may involve the addition of some chemical agents or lime to achieve an ideal pH level, as well as
166 temperature and fluid flow modifications, depending on the type of technique utilized. Moreover,
167 post-operational processes can show a discrepancy but predominantly include dewatering, solid
168 precipitates separation, transporting the solid waste to a landfill, as well as further treatment of the
169 residual fluid till a suitable set of provisions is attained that sanctions it to be reverted to nature
170 (Bhojwani et al., 2019; Ijanu et al., 2020). The formation of secondary pollutants in case of
171 chemical precipitation, fouling and susceptibility by organic matter in the case of membranes, a
172 limited ion removal margin, and a high energy cost in the case of electro-kinetic remediation are
173 all obvious drawbacks in traditional wastewater treatment. Adsorption has showed promise among

174 all existing technologies due to its speedy operation and simplicity, specifically with the
175 development of adsorbents that eliminate the requirement for secondary contaminant and
176 processing. Eternally more and more inorganic and organic materials are being documented as
177 potential adsorption mediators for the removal of toxic metal, such as activated carbon, rice husk,
178 various bacterial species, palm fiber, chitosan, eggshells, clay, clinoptilolite, plants, and different
179 types of nanomaterials (Nghah et al., 2011; Lim et al., 2018; Sherlala et al., 2018). Among them
180 nanoparticles, whether inorganic or organic, have the most outstanding adsorption properties of all
181 existing adsorbents, and some of them are already being used in the wastewater management
182 business. In comparison to other adsorbents or chelating agents, the nanomaterials offer greater
183 efficiency in handling the toxic metal pollutants. This high efficiency in remediating the metal
184 based pollutants owes from the fact that the nanoparticles have high surface area and unique
185 surface properties (Lim et al., 2018). Their surface characterization via different activation
186 processes may enable harmful metal selectivity, allowing for future recycling of these particles
187 rather than their disposal as toxic waste. The metal-organic frameworks (MOFs), Zeolites,
188 bacterial exopolysaccharide, ceramics, algae, and carbons are examples of such type of
189 nanomaterials. Activated carbon is the most extensively utilized nanomaterial in wastewater
190 management, despite being a somewhat expensive choice (Skouteris et al., 2015; Dias and Petit,
191 2016; Gupta and Diwan, 2017; Ahmadijokani et al., 2021). Future 2D nanostructures are rapidly
192 improving in this ever-growing category because they have higher adsorption abilities due to their
193 large functionalized surfaces with unique features that allow them to be integrated into a variety
194 of wastewater treatment processes, either as adsorbents, catalytic and/or antibacterial agents, or
195 functional membranes. The technique is still developing, and facing a number of issues in
196 immediate commercialization of these materials. These drawbacks involve their short life span and

197 incompetent integration in the existing architecture of wastewater management systems (Rasool
198 et al., 2019).

199 **3.1. Effect of pH**

200 The pH of the medium mainly effects the charge density and degree of ionization of the adsorbent
201 and greatly affect the removal of metals. As at higher pH, hydroxide of metals are formed in the
202 form of salts and become precipitate out from the system. This dependency mainly depends on
203 element of adsorbent and chemistry of solution. The zeta potential measurements of MXene shows
204 high charge density at pH lower than 2.41. In this way, the surface of the adsorbent can be
205 negatively charged, positively charged or become neutral depending pH of the system.

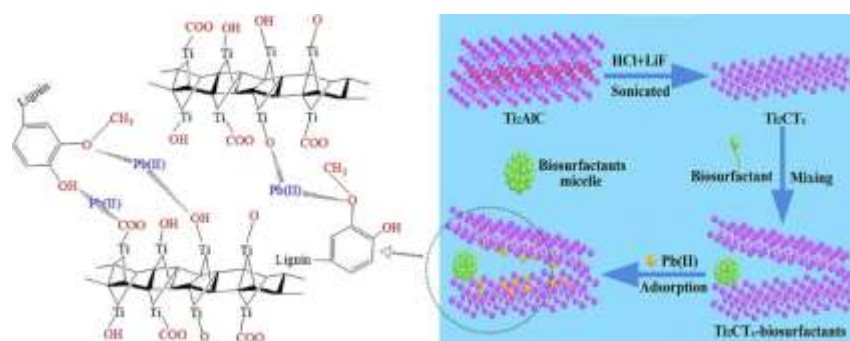
206 **4. MXene and MXene based composites for Toxic Metal Removal**

207 **4.1. Removal of Lead by MXene and MXene based composites**

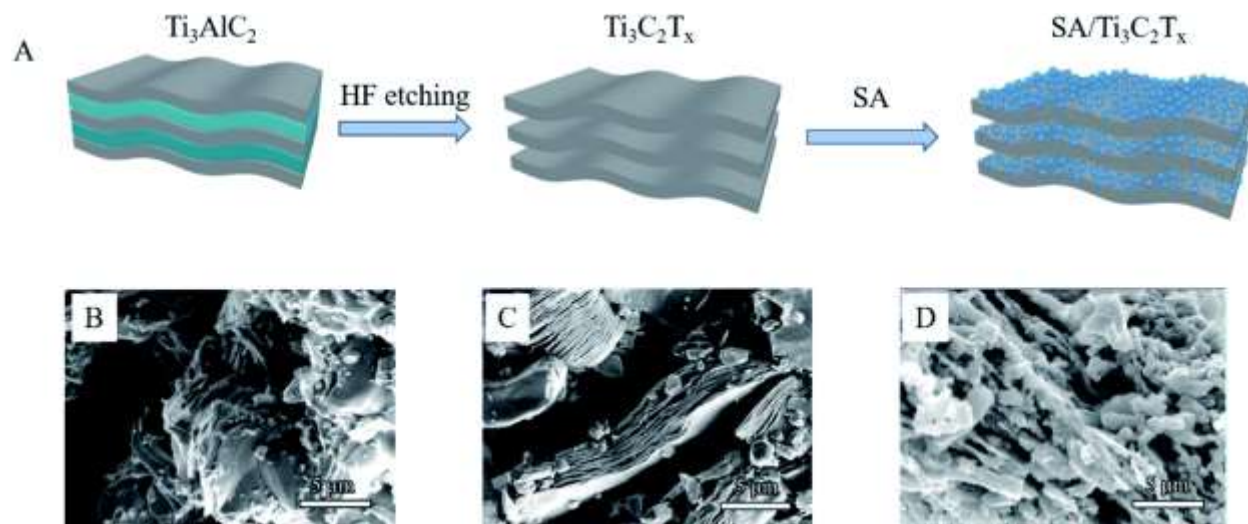
208 Lead is toxic metal that is produced from agricultural and industrial processes. High concentration
209 of lead in aqueous matrices destroys the health of living beings. Peng and his colleagues used 2-D
210 alkylated MXene ($\text{Ti}_3\text{C}_2(\text{OH}/\text{ONa})_x\text{F}_{2-x}$) to adsorb Pb (II) from aqueous matrices in 5% sodium
211 hydroxide solution for intercalation of sodium ions (Peng et al., 2014). Successful intercalation of
212 sodium ions took place and they lead to expand the space among layers which enhanced the rate
213 of diffusion of area which may react with Pb(II) ions. Significant adsorption of Pb (II) (140 mg/g)
214 was observed and equilibrium was attained in 120s. The mechanism involved in this study was ion
215 exchange. Presence of various elements like Ti, F, Na, O, and Pb was confirmed through elemental
216 analysis and it was proposed that intercalated H^+ and Na^+ ions attached to Ti-O (negatively charged
217 species) could exchange with Pb(II) (Giammar et al., 2007). Lead sorption on MXene flakes was
218 found pH dependent and maximum adsorption was obtained in pH range of 5-7 ensuring ion

219 exchange as mechanism of action. At low pH values, MXenes showed less affinity towards Pb(II)
220 ions which assist in regeneration of used MXene in acidic media. MXene material retained
221 selectivity towards Pb (II) ions with efficacy of 95.2%. Jun and his colleagues used the MXene
222 ($\text{Ti}_3\text{C}_2\text{T}_x$) for removal of Pb(II) ions. MXene showed efficient adsorption and it was explained
223 through pseudo-second-order kinetic and the Freundlich isotherm models and equilibrium was
224 obtained in 30 min. MXene exhibited excellent reusability until four cycles (Jun et al., 2020a). Gu
225 and his colleagues synthesized two different MXenes named e-TACFs and e-TACSs through
226 hydrothermal method. e-TACFs and e-TACSs showed maximum adsorption of lead ions 284.9
227 and 218.3 mg/g respectively. Ion exchange and complexation were found as mechanistic way of
228 interaction of lead ions with MXenes which enhanced the adsorption potential. DFT studies
229 supported the results (Gu et al., 2018b). The $\text{Ti}_3\text{C}_2\text{T}_x$ powder contains great ion exchange potential
230 but they show poor adsorption of heavy metals. Du and his colleagues overcome this drawback by
231 regulating $\text{Ti}_3\text{C}_2\text{T}_x$ powder with silane coupling agent (KH570) and they were found efficient for
232 removal of lead ions. The modified powder possessed great surface area, thermal stability and
233 good ion exchange potential. The $\text{Ti}_3\text{C}_2\text{T}_x$ -KH570 powders showed adsorption potential of 147.29
234 mg/g of Pb(II) ions while adsorption potential of pristine $\text{Ti}_3\text{C}_2\text{T}_x$ powder was only 48.28 mg/g.
235 hydroxyl groups of internal MXene were found responsible for adsorption of lead ions. The lead
236 ions adsorption was dependent on availability of hydroxyl and carbonyl moieties of MXenes and
237 KH570 respectively. Thus modified MXenes may be promising for removal of lead ions (Du et
238 al., 2019). Similarly, in a latest study, Ti_2CT_x MXene sheets were functionalized with three
239 different biosurfactants as chitosan, lignosulfonate and enzymatic hydrolysis lignin. The
240 enzymatic hydrolysis lignin functionalized MXene showed high adsorption (232.9 mg/g) of Pb(II)
241 ions and this may be attributed to prevention of Ti_2CT_x nanosheets from restacking and

242 incorporation of active functional moieties in MXene nanosheets due to enzymatic hydrolysis
243 lignin biosurfactant (Figure 2) (Wang et al., 2020b). MXene has limited adsorption potential for
244 metal ions and this may be because of limited adsorptive active sites. Dong and his colleagues
245 synthesized MXene/alginate nanocomposite for adsorption of lead from aqueous solution (Figure
246 3). This synthesized composite enhanced the adsorption potential and chelation capacity of Pb (II)
247 ions. Maximum adsorption of Pb (II) was found to be 382.7 mg/g and equilibrium was reached
248 within 15 mins. MXene/alginate composite can be regenerated with facile acid treatment without
249 loss in activity. So this study showed that composites of MXenes may open new dimensions for
250 high adsorptive removal of heavy metals with high efficacy at low temperature (Dong et al., 2019b)
251 (Table 1).



253 **Figure 2:** Biosurfactant functionalized Ti_2CT_x MXene for adsorption of Pb(II) ions (Wang et al., 2020b)



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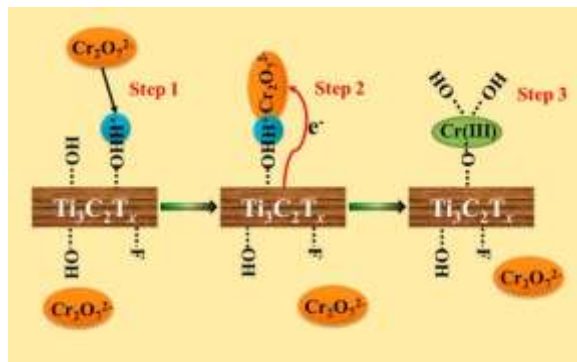
255 **Figure 3:** (A) Schematic of the preparation of the MXene/alginate composites; (B) surface morphology of Ti_3AlC_2 ;
 256 (C) surface morphology of $Ti_3C_2T_x$; (D) surface morphology of the MXene/alginate composites (Dong et al., 2019b).

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258 **4.2. Reduction and Removal of Chromium Ions by MXene and MXene based composites**

259 Chromium is toxic metal that is produced from different industries. Chromium may exist in
 260 trivalent or hexavalent forms. Hexavalent chromium is carcinogenic. MXenes are known for
 261 adsorption of high valent metal ions. Ying and his colleagues employed MXene nanosheets
 262 ($Ti_3C_2T_x$) for adsorption of Cr(VI) (Ying et al., 2015). MXene nanosheets efficiently adsorbed the
 263 chromium metal ions with adsorption potential of 250 mg/g. Below pH 2, Cr(VI) were adsorbed
 264 on positively charged nanosheets (due to presence of hydroxyl moieties) then hexavalent chromium
 265 would reduce to trivalent chromium via electron transfer (Figure 4). Increase in pH would weaken
 266 the electrostatic force of interactions, until pH reaches 13 and it stops completely. On contact with
 267 MXene sheets the chromium metal is reduced with assistance of H^+ ions and precipitates (pH 4.8)
 268 and full precipitates are obtained at pH 5.6 where trivalent chromium may bind to MXene surface
 269 in covalent manner via titanium oxide sites with 98% removal potential. Sheets may be degraded
 270 after use Urchin like rutile MXene based TiO_2-C/TiC nanocomposites were fabricated and they

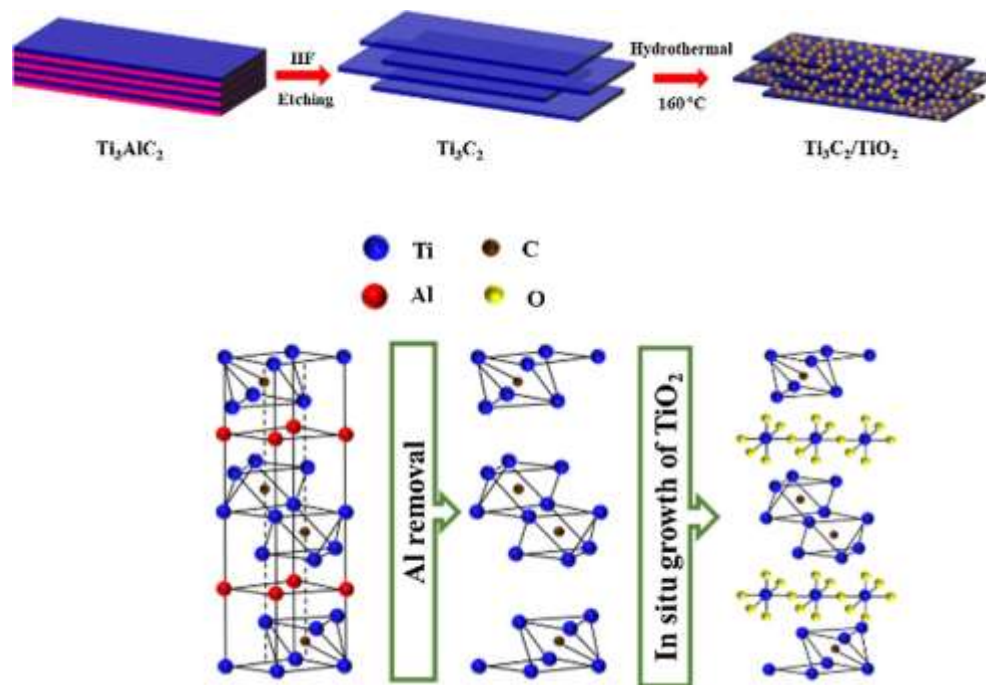
271 showed high adsorption of Cr (VI) with adsorption potential of 225 mg/g (Zou et al., 2016). MXene
 272 flakes were used by group of scientists to adsorb chromium with adsorptive potential of 80 mg/g
 273 at room temperature (Tang et al., 2018).



274
 275 **Figure 4:** Illustration of the removal mechanism of (a) Cr(VI) by the Ti₃C₂T_x nanosheets. Reprinted with
 276 permission from Ref. (Ying et al., 2015)

277 The Ti₃C₂/TiO₂ composite attained effective removal of Cr(VI) from K₂Cr₂O₇ solution. The
 278 mechanism involved is reduction of hexavalent chromium to trivalent chromium and then
 279 adsorption of produced Cr (III) ions (Wang et al., 2020a). After synthesis of MXene flakes the
 280 hydrogen fluoride was employed as etchant and obtained Ti₃C₂ was heated hydrothermally to
 281 grow Ti₃C₂/TiO₂ particles (Figure 5). The 24 h hydrothermal treatment gives optimum Cr (VI)
 282 adsorption with reduction efficacy of 99.35%. Karthikeyan and his colleagues used 2D MXenes
 283 for removal of Cr(VI). The removal rate of Cr (VI) was quick and reaction followed the second
 284 order kinetics. Maximum adsorption capacity of Cr (VI) was found to be 104 mg/g. The MXene
 285 sheets were regenerated by using 0.1 M sodium hydroxide solution. Adsorption phenomena
 286 involved were electrostatic, complexation, surface interaction and ion exchange for uptake of Cr
 287 (VI) ions (Karthikeyan et al., 2021) Recently amino functionalized MXenes (NH₂-Ti₃C₂T_x) were
 288 synthesized. Amino moieties and Ti₃C₂T_x sheets show synergistic effects in adsorption and
 289 reduction of Cr (VI). The NH₂-Ti₃C₂T_x showed maximum adsorption potential of 107.4 mg/g for

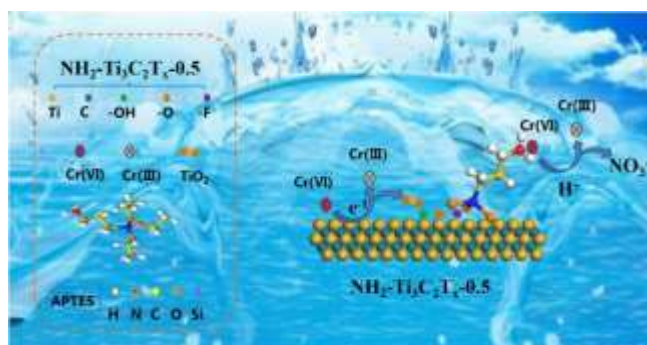
290 Cr(VI) (Kong et al., 2021). Ti (II) and NH_3^+ oxidized in Ti(IV) species and NO_3^- during the
291 removal of Cr(VI). Amino functionalized MXene sheets showed great reusability and selectivity
292 (Figure 6). Khan and his colleagues synthesized MXene and $\delta\text{-MnO}_2/\text{MXene}$ hybrid through
293 hydrothermal method for adsorption of Cr (VI). The pseudopseudo-second-order model was
294 followed. Adsorption of Cr (VI) was pH dependent. MXene and $\delta\text{-MnO}_2/\text{MXene}$ hybrid showed
295 maximum efficiently adsorbed the Cr (VI) with adsorption potential of 273.1 mg/g and
296 353.87 mg/g respectively. The hybride of MXene with transition metal oxides showed highest
297 adsorption potential and this may provide opportunity to remove heavy metals with efficiency due
298 to electrostatic interactions (Khan et al., 2021). Composite of MXene with PEI modified sodium
299 alginate aerogel was synthesized for removal of Cr (VI). MXene/PEI modified sodium
300 alginate aerogel efficiently adsorbed the Cr (VI) with adsorption potential of 538.97 mg/g. The
301 pseudo-second-order kinetic and Langmuir isotherm was followed. The composite strength was
302 enhanced due to polymeric alginate and PEI. And composite showed efficiency uptill five cycles
303 (Feng et al., 2021). Recently imidazole-MXene composite ($\text{Ti}_3\text{C}_2@\text{IMIZ}$) were fabricated and it
304 was used to remove Cr(VI) from medium. During adsorption, the Cr (VI) was converted to Cr (III)
305 and removed through physical adsorption phenomena (electrostatic force of interaction). The
306 composite was reproduce after use (Figure 7) (Yang et al., 2021) (Table 1). From reported work,
307 it can be easily concluded that MXene composites are more suitable and efficient for removal of
308 heavy metals in comparison of pristine MXenes.



309

310 **Figure 5:** Schematic illustration of the preparation of Ti_3C_2/TiO_2 composite. Adapted and reproduced with permission

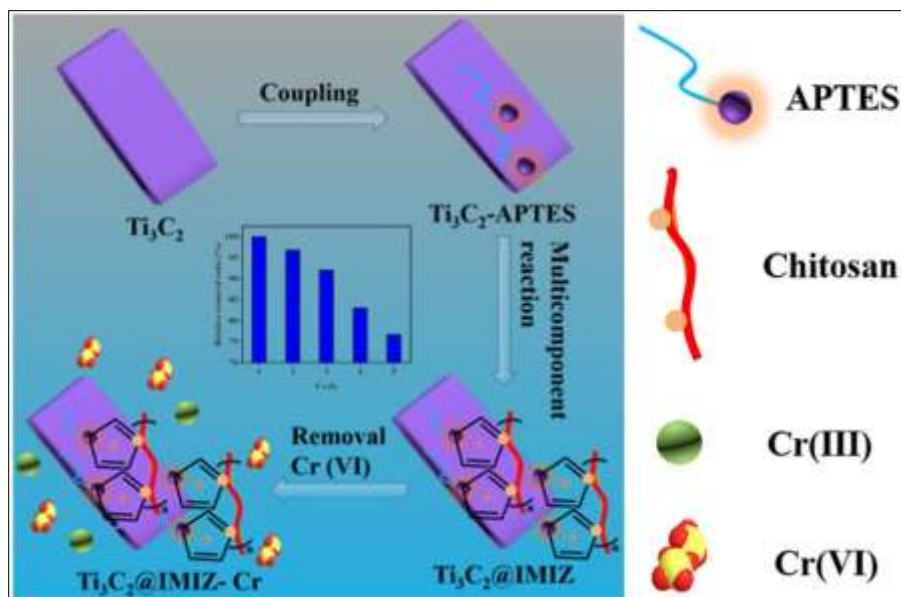
311 (Wang et al., 2020a).



312

313 **Figure 6:** Amino-functionalized MXenes for efficient removal of Cr(VI) (Kong et al., 2021)

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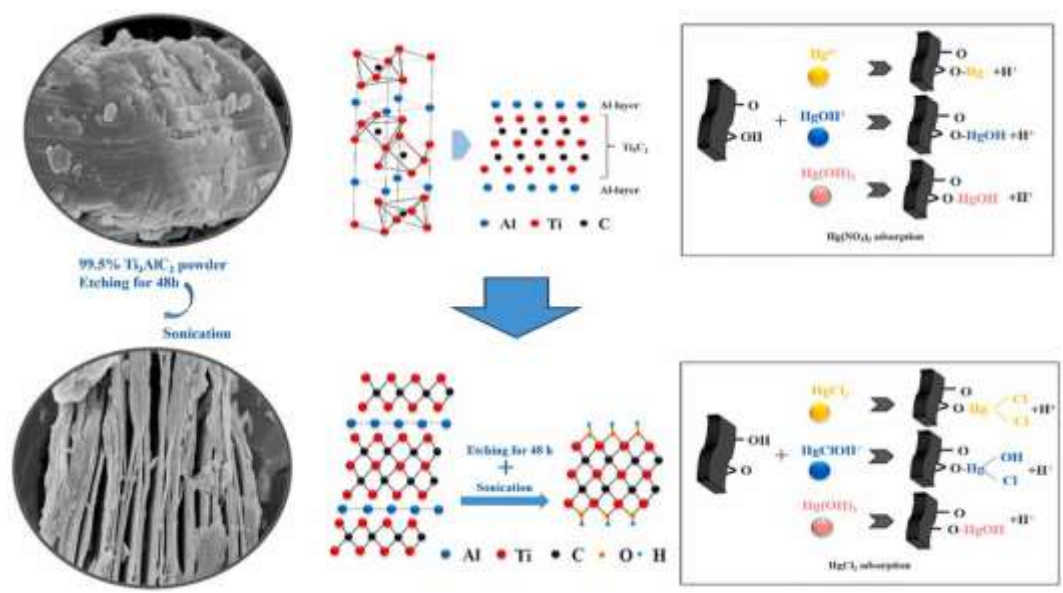
316 **Figure 7:** Synthesis and efficiency of Ti₃C₂@IMIZ for adsorptive removal of Cr(VI) (Yang et al., 2021)

317 **4.3. Removal of Mercury by MXene and MXene based composites**

318 Mercury pollution occurs due to burning of coal, waste materials. Various industries (cement,
 319 paper and mining) are also responsible for mercury pollution. Mercury ions accumulate in human
 320 body and cause severe health problems. Various studies have been conducted for removal of
 321 mercury by using MXene base materials. In a study modified MXene flakes were used to adsorb
 322 Hg (II) at different pH conditions. MXene flakes adsorbed the Hg (II) with adsorption potential of
 323 1128.41 mg/g (Shahzad et al., 2018). MXene flakes were modified by magnetizing them to
 324 enhance their stability and fast recovery. In another study compositing of MXene aerogel spheres
 325 (Ti₃C₂T_x) was carried out with varying concentrations of sodium alginate and this composite (MX-
 326 SA) was used for removal of mercuric ions. High porosity, surface area and oxygenated
 327 functionalities of MXene composite made it eligible to adsorb high amount of Hg(II). The MX-
 328 SA_{4:20} spheres showed exceptional adsorption potential of 932.84 mg/g for Hg(II) while MX-

329 SA_{2:20} also adsorbed the Hg(II) (365 mg/g). This composite showed excellent results at various pH
 330 conditions (Shahzad et al., 2019). Shahzad and his colleagues fabricated the molybdenum-
 331 disulfide functionalized MXenes (MoS₂/MX) for removal of Hg(II) ions. Synergistic effect of
 332 sulfur and oxygenated MXene assisted to obtain highest adsorption of Hg ions with adsorption
 333 potential of 1435.2 mg/g (Shahzad et al., 2020). This composite worked under both acidic and
 334 basic media. This study exhibited that heterogenous composites can be used to remove heavy
 335 metals. Fu and his colleagues employed multilayered Ti₃C₂O_x MXene for removal of Hg (II) with
 336 adsorption potential of 4806 mg/g (Fu et al., 2020). In another study, MXene was used to adsorb
 337 Hg(II) from solutions containing mercuric nitrate and mercuric chloride. From mercuric nitrate
 338 and mercuric chloride solution, 1057.3 mg/g 773.29 mg/g Hg(II) was adsorbed by MXene
 339 material at temperature 30 °C (pH 5). Even at low pH values adsorption potential was maintained
 340 (Figure 8) (Hu et al., 2021) (Table 1).

341



343 Figure 8: Efficiency of oxygen-containing MXene for removal of Hg(II) from solution of mercuric chloride and
344 mercuric nitrate (Hu et al., 2021).

345 **4.4. Removal of Copper Ions by MXene and MXene based composites**

346 MXene based materials have been used for removal of copper. Exfoliated MXene nanosheets were
347 synthesized through ultrasonication under nitrogen atmosphere. $Ti_3C_2T_x$ showed great efficacy for
348 copper removal because of large surface area, porosity, hydrophilicity and novel structural
349 features. The adsorption occurs at oxygenated functional moieties on surface of MXene which
350 assists in reduction of Cu(II) ions and forming CuO_2 , CuO species. The delaminated MXene
351 showed adsorption capacity around 78.45 mg/g of copper (Shahzad et al., 2017). Surface oxidation
352 of MXenes take place after and before adsorption of copper ions. Adsorption of copper was found
353 pH dependent. As low adsorption occurs at low pH values. After completion of adsorption, the
354 MXene flakes showed no regeneration ability. Dong and his colleagues synthesized the hydrochar-
355 wrapped MAX based nanofiber composites. The synthesized composites showed potential for
356 removal of copper ions (Dong et al., 2019a). Recently rutile $TiO_2@d-Ti_3C_2T_x$ hybrid has been
357 used for adsorption of Cu (II) ions with maximum adsorption potential of 95 mg/g (Elumalai et
358 al., 2020). Likewise MXenes ($Ti_3C_2T_x$) functionalized with levodopa (DOPA) showed higher
359 adsorption potential of Cu (II) ions with adsorption potential of 18.36 mg/g (Gan et al., 2020).
360 Composite of MXene with sodium alginate also achieved high adsorption of Cu (II) ions with
361 adsorption potential of 87.6 mg/g and equilibrium was reached in 15 minutes (Dong et al., 2019b).
362 So MXene composites may be highly valuable for removal of heavy metals in comparison of virgin
363 MXene (Table 1).

364 **4.5. Removal/Extraction of Barium by MXene and MXene based composites**

365 Barium is a white shiny metal exist in environment in the form of different compound. It mainly
 366 presents as barium oxide, barium sulfide, barium nitrite and barium halide. The oxidation of
 367 barium produce hydrogen in water and become soluble in water species.

368 **Table 1: MXene and MXene based nanomaterials for removal of heavy metal ions**

Sr #	MXene	Targeted metal	Adsorption capacity	Mechanism	References
Removal of Lead ions					
1	e-TACSs e-TACFs	Pb(II)	218 mg/g, 284.9 mg/g	Adsorption	(Gu et al., 2018a)
2	Ti ₃ C ₂ (OH/ONa) _x F _{2-x}	Pb (II)	140 mg/g	Adsorption	(Peng et al., 2014)
3	Ti ₃ C ₂ T _x	Pb(II)	36.6	Adsorption	(Jun et al., 2020a)
4	MXene/alginate nanocomposite	Pb(II)	382.7 mg/g	Adsorption	(Dong et al., 2019b)
5	Ti ₃ C ₂ T _x -KH570	Pb(II)	147.29	Adsorption	(Du et al., 2019)
6	Enzymatic hydrolysis lignin functionalized Ti ₂ CT _x MXene	Pb(II)	232.9 mg/g	Adsorption	(Wang et al., 2020b).
7	MAX@titanate	Pb(II)	328.9 mg/g	Adsorption	(Gu et al., 2019)
8	AlkMXene-NH ₂	Pb(II)	384.63 mg/g	Adsorption	(Zhang et al., 2020)
Removal of chromium ions					
9	Ti ₃ C ₂ T _x MXene nanosheets	Cr (VI)	104 mg/g	Adsorption	(Karthikeyan et al., 2021)
10	NH ₂ -Ti ₃ C ₂ T _x	Cr (VI)	107.4 mg/g	Adsorption	(Kong et al., 2021)
11	nZVI-Alk-Ti ₃ C ₂ composites	Cr (VI)	194.87 mg/g	Adsorption	(He et al., 2020)
12	MXene	Cr (VI)	273.1	Adsorption	(Khan et al., 2021)
13	δ-MnO ₂ /MXene	Cr (VI)	353.87 mg/g	Adsorption	(Khan et al., 2021)

14	MXene/PEI modified sodium alginate aerogel	Cr (VI)	538.97 mg/g	Adsorption	(Feng et al., 2021)
15	MXenes/TiO ₂	Cr (VI)	49.67 mg/g	Adsorption	(Wang et al., 2020a)
16	Ti ₃ C ₂	Cr (VI)	28.3 mg/g	Adsorption	(Tang et al., 2018)
17	Ti ₃ C ₂ T _x -based films	Cr (VI)	84 mg/g	Adsorption	(Xie et al., 2019)
18	Ti ₃ C ₂ @IMIZ	Cr (VI)	119.5 mg/g	Adsorption	(Yang et al., 2021)
19	Fe ₃ O ₄ @MXene	Cr (VI)	70.2%	Adsorption	(Yang et al., 2020)
20	Ti ₃ C ₂ T _x /PmPD-5/1	Cr (VI)	540.47 mg/g	Reduction/adsorption	(Jin et al., 2020)
Removal of mercury ions					
21	Magnetized MXene flakes	Hg (II)	1128.41 mg/g	Adsorption	(Shahzad et al., 2018)
22	MX-SA _{4:20} MX-SA _{2:20}	Hg(II)	932.84 mg/g 365 mg/g	Adsorption	(Shahzad et al., 2019)
23	MoS ₂ /MX	Hg(II)	1435.2 mg/g	Adsorption	(Shahzad et al., 2020).
24	Ti ₃ C ₂ O _x MXene	Hg(II)	4806 mg/g	Adsorption/reduction	(Fu et al., 2020)
25	MXene	Hg(II)	1057.3 mg/g from mercuric nitrate and 773.29 mg/g from mercuric chloride	Adsorption	(Hu et al., 2021)
Removal of copper ions					
26	Delaminated Ti ₃ C ₂ O _x MXene	Cu (II)	78.45 mg/g	Adsorption	(Shahzad et al., 2017)
27	hydrochar-wrapped MAX based nanofibers	Cu (II)	-	Adsorption	(Dong et al., 2019a).
28	Amino acids modified MXenes (Ti ₃ C ₂ TX-PDOPA)	Cu (II)	18.36 mg/g	Adsorption	(Gan et al., 2020)
29	MXene/alginate composites	Cu (II)	87.6 mg/g	Adsorption	(Dong et al., 2019b)

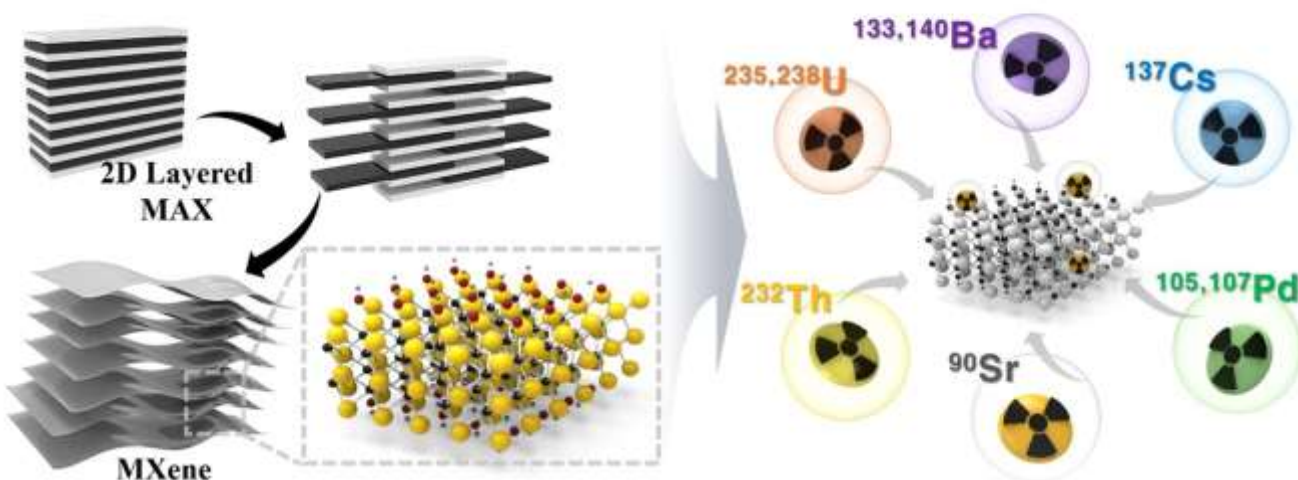
30	TiO ₂ @ <i>d</i> -Ti ₃ C ₂ T _x hybrid	Cu (II)	95 mg/g	Adsorption	(Elumalai et al., 2020)
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370 The compatibility with water make them spread on larger area and affect human and aquatic life
371 (Ghaemi et al., 2011; Torab-Mostaedi et al., 2011). The limit of barium in water is set as 2 mg/L
372 and 0.7 mg/L by USA EPA and WHO respectively (Edition, 2011). So, the presence of barium
373 above this limit cause liver problem, increase in blood pressure, irritation in stomach, difficulty in
374 breathing, heart rhythm change, swelling of brain, muscle weakness, kidney and heart damage and
375 may act as a carcinogenic (Celebi et al., 2009). The main source of barium is oil and gas plants.
376 To remove barium and its compounds, a number of method have been used include ion exchange,
377 precipitation method, adsorption and membrane filtration (Fu and Wang, 2011; Kondash et al.,
378 2014; Fard et al., 2016). Among them, adsorption is low cost, flexible and highly efficient method
379 which is widely used to remove barium contaminants. A number of adsorbent have been
380 established in this regard such as natural dolomite, chloriteillite, carbon based adsorbent, kaolinite
381 and MXenes (Fu and Wang, 2011; Fard et al., 2016; Hadi et al., 2016). MXenes are highly efficient
382 material with good capacity and economic benefits. In 2017 Fard and coworkers established
383 MXene with HF solution and washed through dispersion by sonication in ethanol. The final
384 product obtained by freeze-dried method of washed material for overnight. The MXene is
385 synthesized by intercalation and exfoliation of titanium (III) carbide (II) (Ti₃C₂T_x). In order to
386 study the barium removal, they used this MXene as an adsorbent and with adsorption capacity 9.3
387 mg/g with 100 % removal efficiency. The 90 % of barium was removed from the solution in first
388 10 min selectively as compared to other metals present in solution. This adsorption of barium
389 occurs through physisorption mechanism as a secondary route as shown in figure 9. In addition of
390 this, Chemisorption work as a primary route by using functional groups terminated surface with –

391 O, –OH and –F. These functionalities form a chemical bonding with barium ion present in solution
392 and generate barium hydroxide and barium fluoride (Fard et al., 2017). The applications of this
393 MXene is limited in nuclear waste due to their less capacity of barium adsorption. To this end, Mu
394 and his coworkers enhance the surface activity and metal intercalation of ($Ti_3C_2T_x$) in order
395 improve their adsorption capacity by the using NaOH (Mu et al., 2018). Through this treatment c-
396 lattice parameter increased upto (2.09 nm) which improve the surface interaction affinities toward
397 barium in solution. The functional groups anchoring at the surface shows excellent ability to absorb
398 barium upto 46.46 mg/g. This absorption capacity is unpredictable and useful for nuclear waste
399 management. The improvement of absorption capacity through NaOH is an efficient method. In
400 2020 Jun et al. further improve the absorption ability of ($Ti_3C_2T_x$) toward barium and strontium in
401 waste water. They explain adsorption of barium via electrostatic attraction of negatively charged
402 surface of ($Ti_3C_2T_x$). They report an adsorption capacity upto 180 mg/g of barium in solution. The
403 evidence the adsorption of barium through inner-sphere complexation, chemisorption and
404 chemical ion exchange mechanism by FTIR, isothermal study, kinetic study and XPS respectively.
405 The ($Ti_3C_2T_x$) MXene adsorbent can be reused upto four cycles of adsorption and desorption (Jun
406 et al., 2020b).

2D MXene Material for Removal of Radioactive Pollutants



407

408 Figure 9. Schematic illustration of 2D MXene based materials for the removal of radioactive
409 pollutants from wastewater. Reproduced with permission from (Hwang et al., 2020). Copyright
410 2020 Elsevier.

411 4.6. Removal of Palladium by MXene and MXene based composites

412 Palladium is a very versatile and useful materials in the field of electronics, catalysis, medicine,
413 jewelry and dentistry with peculiar chemical and physical properties. The advancement in
414 electronic device enhance the use and amount of palladium (Parodi et al., 2008; Won et al., 2014;
415 Gupta and Diwan, 2017). The main source of palladium is from minerals, ores and waste
416 electronic devices. It is also present in nuclear waste as Pd-107 and Pd-105 produce through the
417 fission of uranium. This nuclear waste contains non-radioactive or less radioactive palladium (Can
418 et al., 2013). To avoid its mixing with drinking water, Pd containing nuclear waste stored by
419 vitrification and liquid containing Pd convert into glassy matrix. However, Pd presence in this
420 nuclear waste can destroy vitrification and form a separate layer. In this sense, removal of Pd from
421 nuclear waste is very important to avoid further contamination with drinking water (Abney et al.,

2014). A number of method has been employed in this direction include extraction, adsorption, precipitation and filtration (Khan et al., 2015; Mu et al., 2019). Among them, adsorption method seems to be efficient and easy due to its low cost, high efficiency and absence of organic solvents during applications. For this purpose, many adsorbents have been applied. Such as lignin, cellulose, carbon black and chitosan were used as inorganic adsorbent. They work with same principle to capture Pd from aqueous media (Kim et al., 2007; Sharma and Rajesh, 2014). Moreover, their low efficiency and high cost limited the applications. Therefore, it was required to design a new type of adsorbent with low cost and high efficiency. In this regard, transition metal carbide and carbontrides (MXene) are useful material produced by etching method. They pose good hydrophilic properties and readily available for water purification and pollutant adsorbent from environment. In 2019, Mu and his coworkers synthesized $Ti_3C_2T_x$ based MXene by treating Ti_3AlC_2 MAX with HF at different conditions. They synthesized this MXene for the removal of Pd from nitric acid media. The d-spacing of as synthesized MXene triggered at different temperature. As the temperature increase the d-spacing also increased. The d-spacing is directly related to adsorption ability of the material. So, MXene synthesized at 45 °C shows high adsorption power as compared to MXene synthesized at 25 °C and 35 °C. The adsorption efficiency is about 184.56 mg/g, which is higher as compare to other inorganic adsorbents due to higher surface area and d-spacing. The author concluded that the synthesis temperature has vital rule on the adsorption power of MXene (Mu et al., 2018).

4.7. Removal of Cesium by MXene and MXene based composites

Cesium-137 is a radioactive isotopes produced during the fission process of uranium and other radioactive metals. The fission process is largely used in nuclear defense and for the production of nuclear energy. Moreover, nuclear destruction such as Fukushima and Chernobyl also produce a

445 large quantity of nuclear waste in environment (Lee et al., 2017; Cali et al., 2018). As produce Cs-
446 137 is a strong beta and gamma emitter with half-life of 30.17 years and become a major problem
447 in nuclear waste (Tan et al., 2018). It is most harmful material due to its high mobility and
448 solubility with water. Due to its same hydration radius with potassium it can replace potassium
449 from human's body and move in the same way pharmacokinetically as potassium. More
450 interestingly, it enters human and animal body through food like water, meet, fishes and plants.
451 This addition in living organism damage the cells and cause cancer (Khan et al., 2019). In order
452 to prevent problem caused by cesium, a number of method has been used for its safe disposal and
453 removal from waste water and nuclear waste. This involve electrodialysis, ion exchange, solvent
454 extraction, chemical precipitation, coagulation and membrane processing. They are less effective
455 and non-economical as a large amount of nuclear waste is produced with the passage of time. On
456 the other hand, adsorption is a useful technique to remove radioactive waste efficiently (Yang et
457 al., 2018). In this direction, newly developed 2D transition metal carbide and nitrides has been
458 employed as adsorbent for nuclear waste (Lei et al., 2015). Khan and his coworkers study the use
459 of $Ti_3C_2T_x$ as a collector of Cs^+ ion from contaminated water through ingestion test. They study
460 the adsorption of cesium in this MXene through Langmuir and Freundlich isotherm. This
461 adsorbent shows maximum adsorption capacity up to 25.4 mg/g as a coherent with Freundlich
462 isotherm. This adsorption capacity obtained in one minute at room temperature. The heterogeneity
463 of the surface with hydroxyl, fluorine and oxygen groups and multilayer adsorption phenomenon
464 of adsorbent revealed in this work. The adsorption mechanism based on the attachment of Cs ion
465 at the interlayer space and pores of adsorbent in the presence of other ion like (Na^+ , Li^+ , K^+ , Sr^{2+}
466 and Mg^{2+}) (Khan et al., 2019). More recently, Jun and coworkers employed adsorption test by
467 using $Ti_3C_2T_x$ MXene for the removal of radioactive isotopes like Cs-137 from nuclear waste and

468 compared the result with activated carbon as an adsorbent. They noticed that the adsorption ability
469 of MXene was about 148 mg/g for Cs⁺ ion as compared to porous carbon shows 80 mg/g. Although
470 porous carbon has 47 times higher surface area as compared to MXene still have less adsorption
471 capacity. This higher adsorption ability of MXene is due to higher negatively charged surface,
472 which shows that, electrostatic interaction plays vital role for the adsorption of Cs⁺ ion. In addition
473 of electrostatic force among adsorbent and Cs⁺ ion, ion exchange mechanism also involved with
474 presence of other cation like (K⁺, Na⁺, Ca²⁺, and Mg²⁺) and organic acid (Jun et al., 2020b).

475 **4.8. Removal of Uranium (U⁶⁺) by MXene and MXene based composites**

476 Uranium is one of the main constituent of nuclear fuel and contaminated the environment with
477 half-life 4.47×10^9 years. It can mix with soil and water during nuclear waste management, mining
478 and reprocessing of nuclear fuel (Yusan and Akyil, 2008; Stewart et al., 2010). There are two main
479 component of uranium present as toxicant U⁴⁺ and U⁶⁺ ions. Among them U⁶⁺ ion greatly affect
480 the environment due to its high solubility in water and high mobility (Schnug and Lottermoser,
481 2013; Pidchenko et al., 2017). To reduce U⁶⁺ ion in aqueous media different type of sorbent has
482 been used include nanoporous polymer, hydrothermal carbon, zeolites, metal oxides and
483 hydroxides, metal phosphates, graphene oxide and its derivative, metal chalcogen, metal organic
484 frameworks, clays and covalent organic framework (Yang et al., 2014; Bai et al., 2015; Lee et al.,
485 2015; Li et al., 2015; Wang et al., 2018). Another way to reduce U⁶⁺ from aqueous media is to
486 convert it from highly soluble U⁶⁺ to sparingly soluble U⁴⁺ (O'Loughlin et al., 2003; Sun et al.,
487 2014) through bacteria, iron sulfide, chemical reductants, zerovalent materials, magnetite and
488 soluble iron material have been investigated. To remove this radioactive waste more efficiently,
489 two dimensional metal carbides and carbontrides known as MXene having permeable reactive
490 barrier, good stability, high removal tendency and good tolerance have been employed (Ghidiu et

491 al., 2014; Anasori et al., 2017). In contrast with others adsorbent MXenes have hydrophilic nature,
492 charged surface, good ion exchange ability, good resistant towards acids and flexible swelling.
493 These characteristics make them attractive candidates for management of environmental toxic
494 materials. A number of reports have been published in the recent years about the removal of U^{6+}
495 ion by using titanium carbide, chromium carbide and vanadium carbide have been investigated
496 extensively. These MXene are used as batch, theoretical and spectroscopic techniques (Wang et
497 al., 2017; Deng et al., 2019; Fan et al., 2019; Wang et al., 2020b; Zhang and Liu, 2020). Among
498 them titanium carbide shows maximum removal capacity about 470 mg/g due to surface
499 complexation with good electrostatic attraction toward U^{6+} ion as compare to vanadium carbide
500 MXene (174 mg/g). Similarly, strong ion exchange ability of titanium based MXene also
501 responsible for uranium uptake. This titanium based MXene also used in the form composites with
502 good reproduction of U^{6+} ion after conversion to U^{4+} ion. The amidoxime group present in MXene
503 also responsible for uranium removal through coordination with uranyl group and established a
504 bidentate chelating complexes. These all peculiar properties of titanium based MXenes make them
505 excellent adsorbent for the removal of U^{6+} ion from nuclear waste. Zhang and his coworkers
506 measured uranyl adsorption of hydroxyl functionalized titanium carbide about 595.3 mg/g through
507 density functional theory. They proposed that uranyl ions attach with deprotonated oxygen rather
508 than protonated oxygen at the surface of MXene in the form of hydroxy group (Zhang et al., 2016).
509 They reported hydrogen bonding as a dominant factor in uranium ion adsorption. On the other
510 hand, adsorption at vanadium carbide MXene is due to -OH, -O, -F groups. Similarly, Wang and
511 his group reduce the radionuclide waste by converting highly soluble U^{6+} into partially soluble
512 U^{4+} . This removal based on sorption-reduction mechanism with uptake ability 470 mg/g (Wang et
513 al., 2018). Deng et al. established a novel heterostructures $Ti_3C_2/SrTiO_3$ based MXene through

514 oxidation of superficial layer of titanium carbide precursor (Deng et al., 2019). They used this
515 MXene on the base of photocatalytic mechanism for the removal of uranium as its oxides.

516 **5. Limitations of MXenes and MXene based composites Regarding Toxic Metal Removal**

517 Despite significant advancements in MXene production, there are a number of drawbacks to using
518 MXenes for the remediation of harmful metals from wastewater, including lower biocompatibility
519 and durability, inappropriate reusability as well as great affinity for aggregation (Ihsanullah, 2020).

520 Furthermore, rational MXene synthesis with controllable and well-defined surface chemistry
521 continue to be a major challenge. There are more than 30 kinds of reported MXenes based
522 compounds, majority of them were predicted theoretically, thus more effort is needed to
523 functionalize and synthesize different varieties of MXene that are well suited for the experimental
524 treatment of wastewater. Likewise, the biocompatibility and cytotoxicity of MXenes should also
525 be investigated prior to use as a wastewater treatment material. Noticeably, water purification
526 research concentrated solely on $Ti_3C_2T_x$ ($T = OH, F, \text{ and } O$), with little attention paid to other
527 MXenes. On the other hand, $Ti_3C_2T_x$ MXene holds trifling interlayer arrangement and have a
528 tendency to restack in aqueous environment, which restrict its extensive use in eradicating toxic
529 metals with great hydrated ionic radii. The surface accessibility, reusability, and stability of other
530 MXenes and $Ti_3C_2T_x$ for remediation of lethal metals from wastewater can easily be upgraded
531 considerably through recombination with carbon derived materials having unique physiochemical
532 characters and greater surface area as well as abundant, cheaper, and stable polymers (Jlassi et al.,
533 2020; Xu et al., 2020). Moreover, the extensive research is yet to be needed related to the use of
534 MXene nano-architectures in eliminating hazardous contaminants and toxic metals from raw
535 wastewater. Also, there must be a detailed comparison between MXenes and other adsorbents such
536 as graphene, nanomaterials, metal-organic frameworks (MOFs), covalent organic frameworks

537 (COFs)and carbon nanotubes etc. to have a clear and broader idea about their roles as removal
538 agents from wastewater.

539 **6. Conclusions and Future Prospects**

540 MXenes are among the most promising 2D layered nano-architectures currently being researched
541 for the remediation of various hazardous environmental pollutants applications, particularly for
542 the heavy metals. In conclusion, we have covered the essentials of MXenes, including their
543 preparation, characteristics and their extensive characterization. Further, the current advancement
544 in the area of environmental remediation for the removal of heavy metals along with their
545 limitations and drawbacks has been discussed. MXenes have been found to have good
546 metals/heavy metals removal capabilities, and their effectiveness appears to be superior to that of
547 other traditionally used 2D materials and other pollutant adsorbents. Undoubtedly, MXenes have
548 emerged as prospective materials for the removal of metals/heavy metals, there are still a number
549 of impediments to overwhelmed and many questions to be answered before they can be used in
550 the field.

551 1. The number of experimentally documented MXenes are limited as compared to the one which
552 are reported through computations/simulations. Except, $Ti_3C_2T_x$ which is extensively been used as
553 a promising candidate for the environmental remediation of organic dyes, heavy metals and other
554 pollutants of the emerging concern, there are a number of MXenes based nano-architectures which
555 are expected to play an emerging role for the purpose. It's important to explore and experimentally
556 synthesize variety of MXenes with adequate functionalization, required physiochemical
557 characteristics, high water stability, and high absorbability for further advancement in
558 environmental remediation. Further, the area of major concern to construct MXenes based
559 materials for environmental remediation should be the structural features such as, Hierarchical and

560 non-layered carbides as well as the exposure of the active metal component. This will be a
561 challenging task to accomplish. Beyond flat films, various morphologies of MXenes, such as
562 nanocages and nanotubes should also be an area of worth investigations for environmental
563 applications. Also, the surface functionalities play key role in elucidating the adsorption ability of
564 MXenes. In comparison to real-time production, the majority of the theoretical models and
565 modeling were done on the assumption that the MXenes have uniform functionalities at the
566 terminals. To acquire full insights into the prediction of experimental circumstances, precursors
567 used to create designed MXenes with desired functional groups, and target pollutants, finite
568 element modeling theoretical simulations and classical MD are extremely essential.

569 2. The adsorption of metals/heavy metals with hydrated ionic radii bigger than the d-spacing
570 between the MXene sheets is limited by the restacking and narrow interlayer spacing of pristine
571 MXenes. To encapsulate the metals/heavy metals, having bigger hydrated radii, this interlayer
572 spacing can easily be adjusted by the introduction of some cross-linker or intercalants. This can
573 easily enhance the adsorption capacity of MXenes.

574 3. It's worth noting that the delamination conditions and surface functionalities are important
575 factors in determining MXenes' adsorption capabilities. Normally, MXenes produced by synthetic
576 methods are functionalized with several termination groups randomly. As a result, developing
577 synthetic techniques and post-treatments is critical in order to establish a homogenous functional
578 group, which is a challenging problem. More crucially, due to the strong reactivity of the surface
579 metal atoms, it is believed that metals/heavy metals removal utilizing non-terminated MXenes
580 including surface metal atoms will be successful, this should be experimentally examined for
581 adsorption applications. As HF is used as an etching agent for the preparation of number of
582 MXenes so, to develop a fluorine free strategy, which is another challenging factor to be addressed.

583 Till now, the most widely exploited methodology for the fabrication of MXenes is top-down
584 method. This technique lacks in controlling the surface termination feature, which is most
585 important parameter in finding the adsorption/removal ability of the synthesized material. This
586 necessitates the development of bottom-up approach to synthesize the MXenes of desirable
587 features

588 4. Given the rapid use and increasing quantity of MXene based materials, the acute toxicity of
589 MXenes and their possible environmental risks should be thoroughly investigated. More study is
590 needed to expand the spectrum of uses for environmentally benign MXenes in environmental
591 remediation. To address the challenges and practical applicability concerning the environmental
592 remediation, the competitive cost comparison between MXenes and other 2D adsorbents like
593 graphene should be considered. Therefore, cheaper synthetic methodologies and MAX phase
594 precursors should be taken into account. Hence, MXenes composed of naturally profuse elements
595 are commended for accomplishing cost-effective environmental applications.

596 5. MXenes can easily be oxidized in the presence of water and degrade under different conditions.
597 Therefore, the evaluation of different solvents towards their stability must be addressed with due
598 care. The introduction of the MXenes to the polymeric matrices can be an option to increase the
599 stability for future environmental applications. Furthermore, the desired functionalities can also be
600 achieved by modifying the surface and manipulating the interlayer spacing via delamination and
601 intercalation.

602 6. After adsorption it is really tedious to separate the MXenes from the solution, which limit them
603 in-field practical utility for the separation of metals/heavy metals from the greater volume of
604 solutions. MXenes can be incorporated into fibers or MXene derived composites having magnetic
605 nano-architectures can be used to overcome this problem.

606 Conclusively, it is pertinent to say that this novel family of 2D materials has immense potential as
607 adsorbents for the removal of metals/heavy metals. We believe that this study will provide a
608 thorough overview of current research on the metals/heavy metals removal application of MXenes,
609 as well as a significant push to further improve these systems for future environmental remediation
610 research, particularly in the area of metals/heavy metals removal.

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614 **Conflict of interest disclosure**

615 The representative authors have no conflict of interest to disclose in any capacity, either competing
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