

Review

MXene: A new revolution in the world of 2-D materials

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Abstract: MXenes have imposed a profound effect on materials science and nanotechnology fields after their discovery in 2011. Theoretical models have predicted more than 100 potential compositions of MXene whereas laboratory-scale synthesis reflects their success of over 40 distinct structures till date. The distinctive properties of MXenes have led to their use for a diverse range of applications, such as energy storage, environmental remediation, electronics, communications, gas and liquid separation and adsorption, biomedical fields, and optoelectronics. The increased interest of researchers in MXenes has led to a wide rise in research publications, showing their growing importance in different scientific domains. In 2024, MXenes had shown wide potential in various areas, including energy storage devices, electromagnetic interference shielding, nanocomposites, and hybrid materials. However, the variations in the choice of precursors, reactor design, cost, synthesis parameters pose several challenges in ensuring the production of high-quality MXenes. The applicability of MXenes continues to broaden as its compositions are continuously accelerating. This review aims is to provide a comprehensive overview of MXene history, its properties, challenges, latest trends, and different applications to highlight its potential and gather new audiences towards this family of two-dimensional materials.

Keywords: supercapacitor; MXene; MAX; synthesis

1. Introduction

MXenes belongs to a novel class of two-dimensional (2D) materials comprising early transition metal carbides and nitrides, discovered first in 2011 [1]. This family of 2D materials is labeled the formula $M_{n+1}X_nT_x$, where M signifies early transition metals, X describes carbon or nitrogen and Tx refers to surface terminations such as fluorine (F), oxygen (O), hydroxyl (OH) [2,3].

The MXene structure is typically comprised of various *n* + 1 layers of M and intercalated with n layers of X, with numerous surface terminations. The selective etching method is used for the synthesis of MXenes that begins with taking a precursor material which is referred to as MAX phase [4]. The hexagonal packed structure of carbides and nitrides describes the layered MAX phase where A group in the periodic table represents the A elements in the MAX phase such as aluminum, gallium or silicon [5]. With the process of etching, delamination and exfoliation, the A-layer atoms in the MAX phase are selectively removed which provides 2D MXene flakes [6]. There are two main forms of MXene out of which is multilayered (ML) powder and the other is a single-flake colloidal solution. In ML-MXenes, the loosely attached MXene flakes are stacked, whereas the colloidal MXenes are prepared by exfoliating ML-MXenes into single-flake dispersions as shown in **Figure 1** [7,8].

Figure 1. Schematic showing the synthesis of single layer and multilayered MXene.

Till date, four distinct compositional MXenes that are synthesized including M2XTx, M3X2Tx, M4X3Tx, and M5X4T^x as shown in **Figure 2**. It demonstrates schematic representations of both old and newly discovered MXene structures.

Figure 2. Schematic representation of successful synthesized MXenes.

Among these, $Ti_3C_2T_x$, which belongs to $M_3X_2T_x$ structure, was the first ever MXene reported in 2011 and it is one of the most widely studied out of all others [1,9,10]. The representation of the $M_3X_2T_x$ structure is shown in **Figure 3**. Thereafter, in 2012, MXenes was structured as defined by M_2XT_x and $M_4X_3T_x$ were identified [11]. In the general formula of $M_{n+1}X_nT_x$, precursor material determines its number of layers [5]. This dependency on MAX phases governs the achievement of thicker MXenes $(M_{n+1}X_nT_X)$ with larger n) or to finding of new chemistries for M and X elements. In 2019, the discovery of the first-ever $M_5X_4T_x$ ((Mo₄V)C₄T_x) MXene happened from a new MAX phase with five layers of M (M_5AIC_4) after the selective etching of aluminum layers [12]. More than 100 successful compositions of MXene are found from the theoretical calculations on MAX phases and MXenes [13]. Researchers have created a wide spectrum of MXene array by varying elements in the

MAX phases by incorporating solid solutions at the M and X sites which allow them to fabricate a diverse array of MXene compositions. In 2012, the synthesis of the first solid-solution MXenes such as $(Ti,Nb)_{2}CT_{x}$, $Ti_{3}CNT_{x}$, and $(Cr,V)_{3}C_{2}T_{x}$, are carried out [11]. Afterward, a lot of studies on other MXene solid solutions are reported later in 2020 [14,15]. Despite random solid solutions, it has been seen that precise stoichiometric ratios of specific combinations of transition metals give birth to doubletransition metal MXenes. This involved in-plane and out-of-plane ordered MXene. In plane category $n = 1$, such as $(Mo_2/3Ti_1/3)CT_x$ [3] whereas in out-of-plane category *n* $= 2$ or 3, such as Mo₂TiC₂Tx and Mo₂T₁₃C₃T_x [16].

Figure 3. Advancement in the MXene family from 2011 to till date.

As shown by Alnoor et al. in their study, for validating MXene structures, its composition and defect distribution, electron microscopy plays a crucial role [17].

Further advancement in the MXene precursor chemistry specifically in the M and X elements has led to the discovery of other MXene compositions and structures. Later on, Nemani et al. [18] used high-entropy MAX carbide precursors: $TiVCrMoAlC₃$ and TiVNbMoAlC₃, for the successfully fabrication of two high-entropy M_4X_3Tx MXenes, TiVCrMoC3T^x and TiVNbMoC3Tx. This innovation of his findings is shown in **Figure 1**, bottom. Additionally, one more research from the same year has reported the synthesis of a high-entropy M_2XT_x MXene [19]. The continued research in highentropy MXenes further expands its potential applications in this rapidly advancing field. Fluorine (F), hydroxyl (OH), and oxygen (O) fall under the functional groups (T_x) in MXene. It has been illustrated from the Density Functional Theory (DFT) study that the electronic and magnetic properties are influenced strongly by the choice of these functional groups [20,21]. This is because the presence of functional groups on MXene surface significantly empower its electromagnetic properties, mainly by changing its electrical structure, that can result in changes such as conductivity, band gap, according to the functional group type. E.g. addition of oxygen (−O) functional groups can sometimes transit MXene from metallic into semiconductor, whereas the other

functional groups including fluorine (−F) can help in maintaining its metallic behavior with outstanding conductivity.

In the research carried out by Bae et al., it has been demonstrated that for accurately predicting the MXene behaviour, the selection of DFT methods is very important as different methods leads to varying results. For instance, the study of 22 different M_2 CT_x MXenes (where M = Sc, Y, La, Ti, Zr, Hf, V, Nb, Ta, Mo, W, and T = O, F) through DFT and four different methods—Perdew-Burke-Ernzerhof (PBE), SCAN, HSE06, and PBE + U has resulted in new magnetic states in V_2CO_2 , V_2CF_2 , and $Mo₂CF₂ [21]$.

A mixture of different surface terminations in experimental studies (e.g., $F = O$, OH), complicates the realization of predicted properties in MXene. However, a study carried out on MXenes in 2020 has successfully resulted in uniform surface terminations [22]. This achievement has proved that the findings of electronic and magnetic properties as predicted by DFT over the past decade can also be attained experimentally. Thus, controlling the MXene properties via surface terminations remains an area of active research which necessitates the further exploration of MXene through both experimental and computational methods.

Compared to other materials, superior performance has been shown by MXenes in the fields of electromagnetic interference (EMI) shielding. If compared with the same thickness, the titanium- based MXenes such as $Ti₃C₂T_x$ and $Ti₃CNT_x$ possesses EMI shielding effectiveness which surpasses even copper and aluminum thin films [23,24]. Further the optimization of MXenes for the EMI shielding properties can be carried out by varying the transition metals used in their composition or by adjusting the number of layers (n), which generally correlates with their electrical conductivity [15]. Furthermore, MXenes combined with polymers are used to create MXenepolymer composites which have been provenly effective in improving EMI shielding capabilities [22]. It has been depicted from the literature that in various polymer matrices, MXenes are increasingly used as

filler materials which reflect its significant recognition among various research domains [25]. Due to their hydrophilic property, it allows MXene to form a bond with hydrophilic polymers such as polydiallyldimethylammonium chloride, polyvinyl alcohol, and polyacrylic acid [25]. In comparison to other materials, properties including surface functionalities, extensive compositional range, high aspect ratios, and large surface area of the 2D flakes provide distinctive advantages to MXenes in polymeric composites. When dispersion of MXenes is carried uniformly within polymer matrices, its thermal, morphological, mechanical, and rheological properties can be significantly improved [25].

The research on MXene-polymer nanocomposites has been seen growing rapidly with over 150 journal articles published between 2018 and 2024, as compared to only 50 articles from 2011 to 2017 [25]. Furthermore, conductive polymers such as poly (aniline), polypyrrole, and polystyrene sulfonate have attracted the attention of researchers for their interactions with MXenes. These nanocomposites of MXenepolymer have potential applications in strain sensors, electromagnetic shields, energy storage devices, and gas sensors [26,27]. Additionally, due to this nanocomposite it has also been investigated that the overall shelf life of MXene has also been improved significantly. Since MXenes are prone to oxidation, the incorporation of MXene flakes

in solid polymer nanocomposites also helps in mitigating oxidation rates, which are initially affected by exposure to air, water, and temperature [28,29].

The most widely studied application of MXene is their electrochemical energy storage [10]. **Figure 4** lists some of the properties of MXene which describes one of the reasons why MXenes shows great efficacy in the field of energy storage and its comparison with traditional materials in terms of the properties is summarized through **Table 1**. Since their electronic and ionic conductivity is very high, they act as an extremely suitable material in batteries and supercapacitors. With the latest advancements in MXene compositions and composites, their energy storage performance has significantly improved [30].

Figure 4. Highlight of various key properties of MXene.

For instance, Organi et al. in their study successfully synthesized a freestanding, ultralightweight, additive-free $Ti_3C_2T_x$ MXene aerogel using unidirectional freeze casting. This study demonstrated that strain resistance up to 50% can be achieved with $Ti₃C₂T_x$ aerogel. Because of the aerogel technology, electrochemical performance, including high specific capacity, excellent rate performance, and outstanding cyclic stability is achieved. During the aerogel fabrication, the flakes restacking problem in MXene is prevented which eliminates the need for electrochemical cycling to achieve maximum capacity. In this study it also has been mentioned that the orientation of 2D flakes within the MXene structure also influenced the mechanical and electrical properties of the aerogels. Thus, the outstanding electro-mechanical properties achieved suggest that these aerogels can act as a promising candidate for high-quality strain sensors [34].

Further Shao et al., synthesized $Ti_3C_2T_x$ MXene because of the property of its hydrophilic nature which enhances the transportation of electrolyte ions in aqueous solution. The performance metrics obtained from this approach showed a specific capacitance of 245 F/g, energy density of 35 Wh/kg, and a power density of 2500 W/kg. These results proved the application of MXene-based electrodes in supercapacitor, especially in aqueous systems where fast ion transfer benefits its energy storage. Traditional electrode materials generally face drawbacks towards ion transportation, energy density, and capacitive performance [35].

Afterwards, a study by Liu et al. showed the introduction of PANI into $Ti_3C_2T_x$ synthesising $Ti_3C_2T_x/PANI$ composite, for improving the specific capacitance to 530 F/g and achieving 52 Wh/kg energy density. The research revealed that with the integration of polyaniline (PANI) the pseudocapacitive behavior is promoted which leads to improving both the capacity and stability that is vital for energy storage applications [36].

Later, research by Zhao explored the modification of $Ti_3C_2T_x$ MXene by Ni(OH)₂, presenting the capacitance of 700 F/g and an energy density of 138.4 Wh/kg. The novelty of this article showed that with incorporating $Ni(OH)_2$ in MXene, it boosts its redox activity thus facilitating higher energy and stability suitable for robust, powerdemanding applications [37].

Feng et al. (2022) presented the development of MXene/carbon nanocomposites for enhancing the performance of fabricated flexible energy storage devices. The research focused on designing a hybrid structure which combined MXene's property of high electrical conductivity with structural stability of nanocarbons. The result forms a hyrid material showing the capability of delivering capacitive value of 380 F/g and an energy density of 47 Wh/kg. The novelty from this study lies in optimizing the configuration of layers such as efficient electron pathways of

MXenes and strength and flexibility of nanocarbon which helped in providing a practical and portable energy storage solutions. This unique strategy possibles the composite material to yield high power density, making it suitable for flexible electronic applications and wearable devices [38]. **Table 2** highlights some more publications showing the comparison of MXene based on their performance metrics:

Material	Capacitance (F/g)	Energy Density (Wh/kg)	Power Density (W/kg)		Cycles References
$Ti_3C_2T_x$ flakes	375	38	8000	10,000	[39]
$Ti_3C_2T_x$ nanofluids	300	33	5000	8000	$[40]$
$Ti3C2Tx/AuNPs$ (Symmetric SC)	696.67	138.4	2076	5000	$[31]$
$Ti_3C_2T_x/PANI@M-Ti_3C_2T_x$ Hybrid	530	52	480	-------	[41]
$Ti3C2Tx$ with graphene	254	35.28	18.14	5000	$[42]$

Table 2. Comparing different MXene compositions based on their performance metrics.

The exceptional mechanical strength, bending rigidity, and control over 2D flake thicknesses of MXene flakes also make them a promising candidate for tribological applications [43]. For example, to improve the antifrictional properties of base oil, the addition of just 0.8 wt% $Ti_3C_2T_x$ did a great job [44]. Huang et al. [43] in their research achieved superlubricity by coating $Ti_3C_2T_x$ MXene on a silicon substrate which resulted in a friction coefficient of 0.0067 ± 0.0017 , that is 3.3 times lower if only silicon substrate is used. This discovery opens new paths for exploring MXene coatings as innovative solid lubricants for various applications.

2. Challenges faced by industries

The massive adoption of MXenes in industries has faced a lot of challenges related to environmental impact and production costs. For efficient synthesis of MXene, selecting an appropriate technique is also very important as it has a huge impact on its production efficiency, quality and cost-effectiveness. From the literature, it has been seen those methods for instance, chemical etching and exfoliation, show different results of MXenes in terms of surface area, morphology, and layer thickness [45]. All these properties are directly linked in affecting the material's electrochemical, mechanical, and thermal performance, which are vital for applications involving energy storage and catalysis. In addition to this, scalability, environmental impact, and economic viability are also affected by the right choice of manufacturing technique. Thus, it is very crucial to optimize these techniques so that desired material properties and production efficiency can be achieved. In **Figure 5** all these challenges related to the production of MXene are illustrated. For the large-scale production of MXene, reactor choice is a crucial parameter as.

Figure 5. Illustration showing various challenges affecting the quality of MXene synthesized .

It impacts material quality, scalability, and cost measurements.

During reactor selection, operational parameters such as temperature, pressure, and mixing are affected, which further influences the chemical and structural properties of MXenes. Further, the design of the reactor should also be chosen in such a way that the yield, production rate, and energy consumption will be in good shape. Thus, to produce MXenes for numerous fields, the choice of reactor plays a pivot role. Additionally, factors such as reactor material composition and safety design are very important in obtaining its overall performance.

It should also be kept in mind that appropriate precursors selection for the right quality MXene is also an important factor crucial for limiting cost and enhancing material quality. The composition and qualities of the final MXene product formed are highly affected by the choice of precursors. To minimize production costs, affordable and easily available precursors can help in this scenario. Additionally, the right quantity of precursor material influences the purity and uniformity of MXenes, which thus results in affecting its capabilities in energy storage devices. However, if the impurities or variations in quantity or quality of precursor are present, it may lead to poor MXene properties, affecting its product quality and reliability. Thus, to carefully balance cost-effectiveness with high-quality MXene, precursor selection plays a crucial role in ensuring the optimal performance and market competitiveness.

Further, the parameter that is also responsible for playing a major role is the consistency in the property of MXene as any variation in this might results in producing inconsistent performance, creating hurdles in fulfilling the requirements of certain applications. This may results in additional testing and controlling the quality measures, further leading to increased production costs. Moreover, flexibility in choosing the material properties will also compromise MXene reliability and effectiveness, and less market acceptance. Thus, it is very important to ensure that the material properties are consistent for optimal product performance, reducing the need for extensive quality control for cost purposes and mitigating waste.

High costs and environmental hazards to raw material pose a significant barrier towards the large-scale production of MXene. To mitigate these issues, changes in chemical usage or precursor materials are carried out. For instance, if transition metal oxides (e.g., $TiO₂$ instead of Ti) are substituted against transition metals, the cost of fabricating MAX phase can be significantly lowered [46]. Furthermore, the usage of low-cost sources of A layer atoms such as recycled aluminum or silicon, and alternative sources of carbon, such as recycled carbon from tires can also help in reducing the cost problems. As aluminum and recycled carbon is abundantly present in scrap and tires globally, they offers lower costs and reduction in greenhouse gas emissions in comparison to traditional sources [46–48].

One of the research carried out by Jolly et al. [33] uses secondary aluminum, titanium dioxide, and recycled carbon from tires for the synthesis of $Ti_3C_2T_x$ MXene from the $Ti₃AIC₂ MAX phase. With this method, MXene exhibited an electrical$ conductivity of 5857 ± 680 S/cm and comparable electrochemical performance in supercapacitors to that of $Ti_3C_2T_x$ MXenes produced by conventional methods. This approach represents a significant step towards

optimizing the environmental impact and cost-efficiency of MXene production. While traditional MXene fabrication methods are already being explored for commercial applications, cost- effective and environmentally friendly production methods have the potential to accelerate the broader industrial application of MXenes. The selection of an appropriate technique for MXene bulk manufacturing is crucial due to its substantial impact on production efficiency, material quality, and costeffectiveness [49]. Various methodologies, including chemical etching and exfoliation, result in MXenes with differing properties such as surface area, morphology, and layer thickness. These properties, in turn, influence the material's electrochemical, mechanical, and thermal performance, which are critical for its applications in energy storage and catalysis.

Moreover, **Table 3** summarizes the application level, advantages, and disadvantages of MXenes in specific industries, including strain sensors, gas sensors, and energy storage devices.

3. Future scope

The improvement in synthesizing MXene is widely dependent on innovative technologies and breakthroughs. Modern reactor designs, precursor choice, optimization of synthesis method, environmental conditions and cost parameters are the major parameters for enhancing the quality and properties of MXene. Further, the industrial-scale production of MXene is highly influenced if the academia and industries collaborate. The results generated by academic research provide insights into its foundation, novel synthesis methods, and the latest material discoveries. Whereas, with industry it shapes it practically in terms of applications and scalability requirements. This vital interaction between academics and industries accelerates the outcomes of research findings to practical applications, thus enhancing production efficiency, minimizing costs, and improving quality. This collaborative ecosystem, driven by the exchange of knowledge and resources between academic and industrial sectors, fosters advancements in MXene manufacturing that are both theoretically robust and commercially viable for diverse applications. Further, the innovative composites of MXene with new materials and MXene composition with its family

members can also revolutionize the industry with the best combination which can result in improved energy storage devices.

4. Conclusion

Ultimately, this review focuses on depicting MXene materials as the pioneers in the area of advanced materials, showing its significant potential in various sectors such as electronics, solar, energy storage, and batteries. However, synthesizing MXene came across various challenges related to maintaining quality, cost, and consistency. Environmental and safety concerns are also addressed within the review. It offers a comprehensive roadmap for researchers, industry professionals, and policymakers, fostering scientific advancements and facilitating the widespread adoption of MXene materials. This collaborative effort between academia and industry is essential for leveraging MXene's capabilities to address contemporary challenges and drive innovation across multiple domains. Since the discovery of MXene in 2011, explosive growth has been witnessed on the research of this 2D material, with over 8300 research articles successfully published in more than 400 journals in 62 countries [59]. The number of published articles has been showing an upward trend, with over 3000 manuscripts alone published in 2022, as compared to 1493 and 226 in 2020 and 2017. This reflects its progressive growth as the increase in material's relevance has broaden the scope of its applications. Additionally, the data from google scholar reveals a sharp rise in interest for "MXene" globally since 2015, aiming to reflect its overall growth in research engagement. The publication surge, combined with the its compositions and glorified online interest, highlights the rapid expansion and immense potential of MXenes across various scientific and industrial fields.

Conflict of interest: The authors declare no conflict of interest.

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