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Review article

# Recent advances in machine learning applications for MXene materials: Design, synthesis, characterization, and commercialization for energy and environmental applications

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ABSTRACT

MXene-based materials are characterized by excellent superconductivity, superb ion-holding capacity, large surface area, and rapid electrochemical reactions, making them viable options for applications in high-capacity energy storage and conversion systems (ESCS) such as portable digital devices, electric vehicles, power transportation, modern intelligent networks, and 5 G telecommunications. This review article looks at the latest developments and some of the difficulties in the synthesis and modification of MXene-based materials and highlights the transformative role of machine learning (ML) in advancing MXene research and applications. Applications in energy storage and water purification are discussed alongside the economic and industrial challenges of large-scale production. Recent studies confirm that ML models have been instrumental in improving MXene synthesis processes, enabling higher yields and optimization of properties, better purity, and scalability through real-time process control and reinforcement learning. Techniques such as genetic algorithms, evolutionary algorithms, and Bayesian optimization accelerate the discovery of novel MXene phases tailored for specific uses. The review identifies future directions in MXene research, emphasizing the development of scalable fabrication methods, ML-driven material informatics platforms, and the expansion of MXene applications in electronics and beyond. By integrating ML, MXene research is poised to achieve faster, cost-effective advancements and commercialization for next-generation technologies.

## 1. Introduction

Materials with high-capacity energy storage/conversion systems (ESCS) are in increasing demand, especially in applications like modern intelligent networks, 5 G telecommunications, power transportation, portable digital devices, and electric cars. As a result, there is an increasing need to develop next-generation ESCS with superior performance [1]. Two-dimensional materials such as MXenes, graphenes, and other metal organic frameworks (MOFs), have garnered interest as potential materials for enhancing electrode/electrolytes performance in energy storage applications. MOFs are characterized by their porous structure, ordered crystal frame, and customizable configuration. Graphenes are new carbon nanomaterial, with carbon atoms existing in two-dimensional (2D) lattice structures [2]. Kumar et al. [3] recently compiled the latest developments in the synthesis, reduction, and exfoliation of graphene-based materials, comparing the differences in the characteristics of their various production techniques. The study concluded that high-quality 2D materials suitable for electrode materials applications can be produced with the help of photon-induced irradiation techniques. The recent advances in vacancy engineering of

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2D materials for energy storage applications (supercapacitors and secondary batteries) have also been an area of great interest and Kumar et al., [4] concluded that vacancy defects can effectively modify the electronic characteristics of 2D materials, enhancing the charge-transfer processes/reactions. There have been a few review articles published that cover recent progress and difficulties in the field of 2D materials' electrochemical energy storage applications [5–7]. These studies mainly focused on the developments and utility of graphene-based materials and metal-organic frameworks for electrochemical energy storage applications.

MXenes are a class of two-dimensional materials that have attracted substantial consideration due to their exceptional properties, including superconductivity, ion-holding capacity, large surface area, and rapid electrochemical reactions due to their unique electronic structures and electrical characteristics [8–10]. MXene materials have been successfully utilized in various fields, including applications in energy storage, catalysis, and electronics [11]. MXenes are generally being researched for a variety of possible applications, such as catalysis, supercapacitors, and anodes in lithium-ion batteries. $Ti_3C_2$-$MoS_2$ composites, for example, were employed as novel gas sensors and had good active surface sites, which made them appropriate for the detection of highly sensitive pollutants. A further advancement, in medical diagnostics is the quick detection of influenza virus and SARS-CoV2 using MXene–-graphene field-effect transistors [12]. With its large surface area as well as excellent thermal conductivity, the conductive carbide core of MXenes' 2D material offers special qualities for sensor applications. It is possible to alter the electronic band filling and, consequently, the location of the 3d or 4d-band by choosing the appropriate transition metal. Additionally, it is possible to modify the surface chemistry of MXenes and optimize different surface interactions. By adding heteroatoms, changing the surface chemistry, or combining MXene with other materials, its properties can be modified to fit certain uses and improve performance in a range of situations [13].

Recently, researchers have been seeking ways to develop a novel class of MXene-based materials with superior properties, optimize MXene materials' properties, and establish a suitable channel for large-scale production of MXene materials [14]. Many authors, including He et al. [15], and Brown et al. [16], have suggested the use of a machine learning (ML) approach as a means of improving the properties, performance index, and production capacity of MXene-based materials. ML algorithms can predict the dynamic nature of MXene materials properties, thereby optimizing their functional properties [17]. This makes the incorporation of ML in developing MXene materials an interesting research topic. Li et al., [12] and Shinde et al., [18] are among the few authors who carried out critical reviews on the chemistry, properties, and applicability of MXene–based materials particularly in electrochemical energy storage. None of these studies considered the aspect of integrating ML approach for novel materials design and superior performance index

It is important to acknowledge that while these materials demonstrate potential, their practical application and integration into machine learning systems remain active research and development areas. Current efforts primarily focus on understanding their behavior, improving their properties, and exploring unique applications within artificial intelligence and machine learning. However, the dearth of detailed literature reviews on the use of ML algorithms in the various applications of the MXenes has motivated the exploration of this area of research. Currently, the most related review article covers a single family of MXenes – the double transition metals (DTM) MXenes [19] and others existing in the prior research explores different aspects of their applications in energy storage, functional properties predictions, catalysis and electronics [9,20,21].

Qian et al. [21] reported on the possibility of using ML in the application of MXenes in batteries, supercapacitors, biology, and catalysis, while Roy et al. [20] predicted the functional properties of MXenes using the ML approach. These studies were based on computational analysis and did not systematically report the applications in energy storage, catalysis, water absorption, and electronics. The comprehensive use of ML algorithm in the various fields of applications of MXenes including electronics has not been reported. This is our motivation for this review.

This review provides a detailed overview of MXene and its use in diverse applications. Subsequently, a thorough analysis is presented in relation to the traditional characterization methods, focusing on the limitations and challenges in service conditions and the roles of machine learning in characterization covers electrical properties, mechanical properties, and thermal stability. Furthermore, this review identifies unique machine learning models that have been applied in predicting the MXenes' properties and the commercial utilization in several fields, including energy storage and water purification applications. Moreover, we addressed the problems and outlooks of MXene materials. This detailed overview also portrays the futuristic research areas that would encourage extensive utilization of MXene products and investigation into ML application in MXene materials.

### 1.1. Overview of MXene materials

Two-dimensional (2D) materials are a relatively new class of engineering materials with extremely high aspect ratios that correspond to the thickness of a few atomic layers. These materials have superior chemical, mechanical, electrical, thermal, and optical capabilities because of their reduced dimensionality and quantum confinement effect when compared to their bulk 3D counterpart [22]. Although two-dimensional (2D) materials have existed for a century, the discovery of graphene in 2004 elevated their significance in materials science to a new level. Since then, a great deal of study has been done on various structures that resemble sheets ranging from single to multiple layer sheets of carbon atoms [6]. Most 2D materials such as MXenes, graphenes, and metal organic frameworks have garnered interest as potential materials for enhancing electrote/electrolytes performance in energy storage applications, catalysis, and electronics [5]. Metal organic frameworks (MOFs) belong to the family of 2D coordination polymeric hybrids made up of metal ions and organic ligands, exhibiting multi-faceted interactions between inorganic and organic components. MOFs have porous structure, ordered crystal frame, high specific surface area, adjustable configuration, non-linear optics, and heterogeneous catalysis. Owing to these unique characteristics, MOFs show a variety of uses in energy storage devices, optoelectronics, biomedicine, and telecommunications engineering [1]. Poor stability, conductivity, and metal leakage concerns are among the drawbacks of MOFs, and their high manufacturing costs and recycling/regeneration challenges are major obstacles to their commercial utilization [1]. Graphenes on the other hand are new carbon nanomaterial, with carbon atoms existing in two-dimensional (2D) lattice structures [2]. Graphenes are characterized by high mechanical strength, flexible structure, superconductivity, and optical transparacy, making them suitable for energy storage applications, catalysis, and electronic devices [23]. Several techniques for producing graphene include mechanical exfoliation, Liquid phase exfoliation (LPE), chemical vapor deposition (CVD), and chemical exfoliation [4]. Margaryan et al., [24] demonstrated the conversion of graphite into graphene using the LPF techniques by the ion intercalation mechanism and joining of graphene flakes as schematically illustrated in Fig. 1.

The recent developments in the synthesis, reduction, and exfoliation of graphene-based materials, comparing the differences in their characteristics based on various production techniques has been reported Kumar et al. [3]. The study concluded that high-quality 2D materials suitable for electrode materials applications can be produced with the help of photon-induced irradiation techniques. Studies have shown that graphenes-based materials are appropriate for energy storage devices and especially for lithium ion batteries (LIBs), owing to their layered structure and the reversible reaction between these materials and the

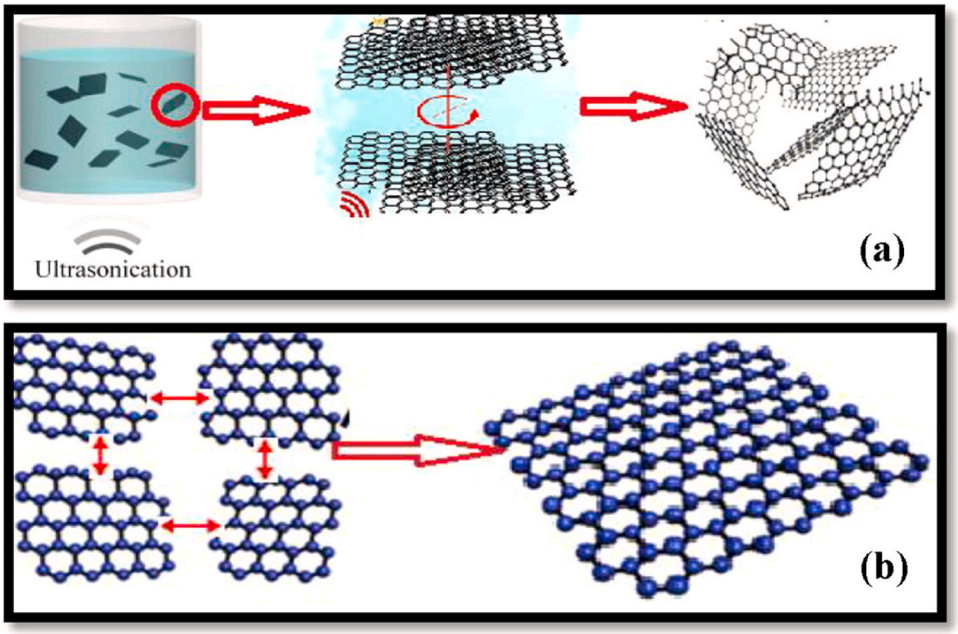



**Fig. 1.** (a) Liquid phase exfoliation, (b) joining of graphene flakes [24]. Culled with permission from Elsevier.

lithium–carbon compounds used as electrolytes, resulting in greater energy density and storage capability [7,23,25]. However, compared to traditional batteries, graphene has a low charge capacity, is expensive to produce, and is challenging to integrate and disperse uniformly in composite electrodes. The high surface area and flexibility of graphene also result in high electrolyte consumption and poor Coulombic efficiency [26]. While research is ongoing to surmount these limitations, new class of 2D materials particularly MXenes are being developed and characterized for superior electrote/electrolytes performance in energy storage applications.

Table 1 summarizes the general characteristics, applicability, and limitations of the various classifications of 2D materials. It can be deduced from Table 1, that 2D-based materials have diverse unique functional characteristics that support their utilization in catalysis, electronic materials devices, electrode materials, structural applications, and energy storage devices. Although graphenes are robust and can be produced through intricate mass production channels, Mxenes have more energy storage capacity and flexible synthesis.

MXenes constitute a group of two-dimensional (2D) materials encompassing transition metal carbides, nitrides, or carbonitrides. These materials were first discovered in 2011 by scholars at Drexel University [29]. This first generation of MXene was created by selectively etching metal layers from the MAX phases of the layered 2D transition metals of carbides and nitrides using hydrofluoric acid [28]. Their nomenclature is derived from their unique structure with M denoting the transition metal, X representing carbon and/or nitrogen, and "ene" signifying their 2D composition [30].

MXene composites are characterized by remarkable properties, including lightweight, flexible structures, high electrical conductivity, and large surface-to-thickness ratio, which make them adapt to diverse applications [31]. Over the past decade, MXenes has emerged as a highly promising class of new material with the potential to substantially advance the course of technology [32]. This advancement is creating new prospects across various domains, even as they are increasingly utilized in electrochemical energy storage devices, including batteries and supercapacitors, environmental remediation, and catalysis [33]. Fig. 2 delineates the structural evolution of MXene materials over about a decade (2011–2021) and quantifies the increase in research interest

**Table 1**
General characteristics, applicability, and limitations of the various classifications of 2D materials.

| 2D Materials | Materials Characteristics | Synthesis process | Cost | Applications |
|---|---|---|---|---|
| Metal Organic Frameworks | MOFs have porous structure, ordered crystal frame, high specific surface area, adjustable configuration, non-linear optics, and heterogeneous catalysis [1] | Synthesized by mixing organic components with metal ions to create a porous, crystalline structure. Methodologies such as mechanochemical synthesis, microwave-assisted synthesis, and electrochemical synthesis have been used to produce MOFs [5]. | High [13] | Li metal batteries, energy storage devices, optoelectronics, biomedicine, and telecommunications engineering [1] |
| Graphenes | Graphenes are single layer of carbon atoms in a hexagonal lattice characterized by excellent mechanical strength, flexible structure, have zero band gap, superconductivity, and optical transparacy. Has low environmental impact [23] | Exfoliation technique (mechanical exfoliation, liquid-phase exfoliation, and chemical exfoliation); plasma etching method; chemical vapor deposition; thermal pyrolysis; epitaxial growth technique; and unzipping of carbon nanotubes (CNTs) among other emerging techniques [2,4]. | High [13] | Energy storage applications, catalysis, electrode materials, and electronics [6] |
| MXenes | MXenes are 2D transition metal carbides/Nitrides with characteristic large surface area, which improves ion-holding capacity; has tunable band gap, superconductivity, which speeds up ion transport; tunable surface chemistry and flexible structures; good electrochemical properties. Good strength. Have potential high environmental Concern depending on method of production [13] | MXenes are typically synthesized by the selective etching of the A-layers in a MAX phase, leaving behind the MXene structure (chemical etching, alkali-assisted hydrothermal etching, molten salt etching etc.). Exfoliation and washing techniques have often been used to synthesize MXene structures [27]. | Low [13]. | Energy storage and electronic devices, electric vehicles and power transportation equipment [18,28]. |

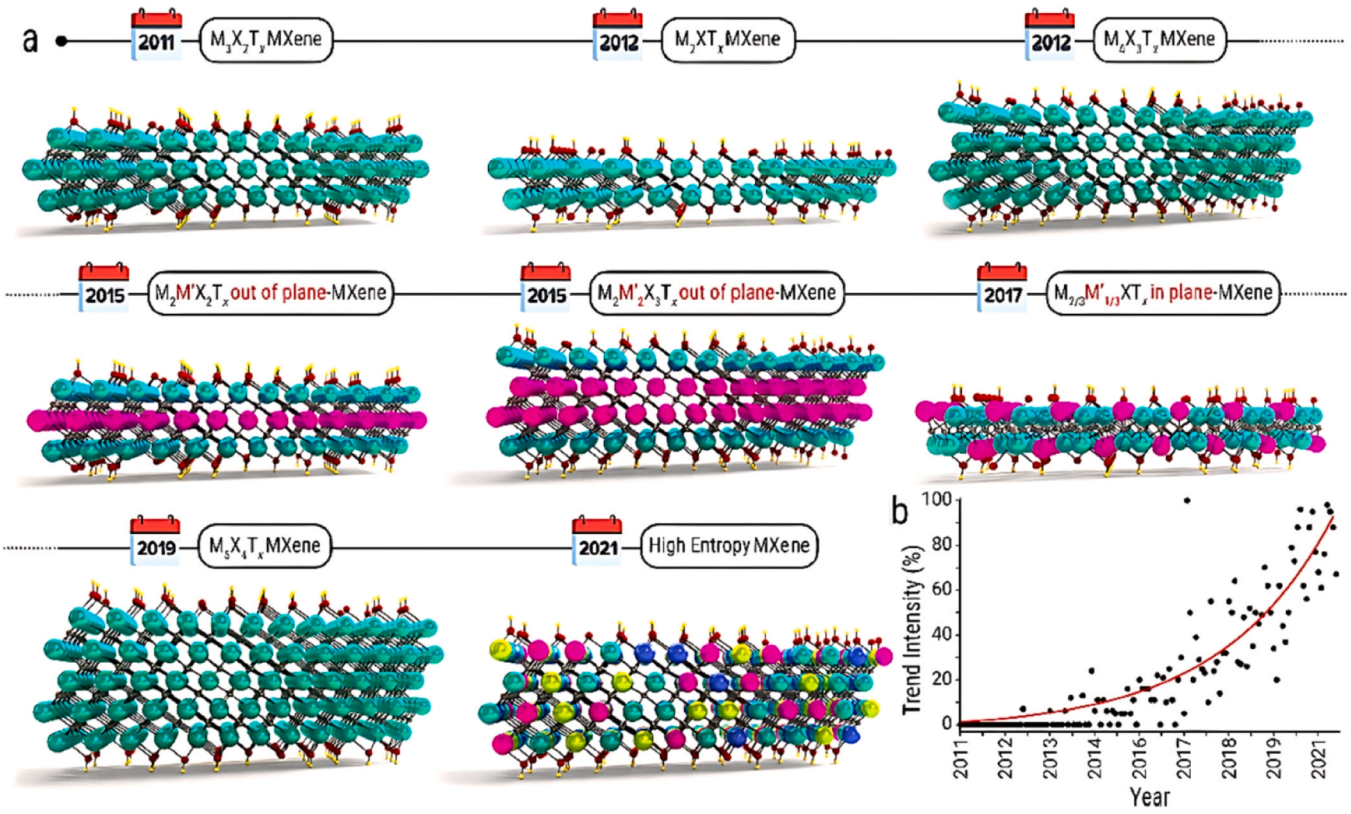



**Fig. 2.** (a) The structures of MXenes. (b) The data collected over the decade from users' engagement with the word "MXene." [34]. Culled with permission from Elsevier.

throughout that timeframe. Fig. 2a illustrates the structural compositions. Researchers have recorded a significant number of experimentally produced MXenes according to their components.

The MAX phase material is another new material recently developed and characterized with a structure similar to MXenes. The MAX phase comprises a transition metal labeled as M, a group of 13 or 14 elements referred to as A, and either carbon or nitrogen, denoted as X. MXenes and MAX phases are similar in composition, with MXenes created through the specific removal of the 'A' phase from a MAX phase material [35]. The selective removal of the 'A' phase from the MAX phase material is possible due to the reduced bonding energy of the 'A' phase to both 'M' and 'X'. This process yields $M_{n+1}X_nT_x$, where T denotes a surface functional group such as -OH, -O, or -F, and the subscript *x* signifies the total number of functional groups. For instance, to create $Ti_3C_2T_x$-type MXene material, hydrofluoric acid (HF) is traditionally used to etch $Ti_3AlC_2$ [36]. The $Ti_3C_2T_x$-type MXene product exhibits high electrical conductivity and has a structure resembling that of an 'accordion' which can be easily separated to yield MXene nanosheets. Due to safety concerns associated with the use of concentrated HF as etching reagent in the synthesis of MXene materials, series of alternative etchants have evolved over the years [37]. These alternative etchants include hydrochloric acid (HCl), and lithium fluoride (LiF) often produces HF bye-products during the synthesis of titanium-based MXenes. Eqs. 1–3 presents the reactions for synthesis of generic MXene from MAX-based phase material such as $M_{n+1}A_lX_n$ using HF-based etchant:

$$M_{n+1}A_lX_n + 3HF = A_lF_3 + 1.5H_2 + M_{n+1}X_n \quad (1)$$

$$M_{n+1}X_n + 2H_2O = M_{n+1}X_n(OH)_2 + H_2 \quad (2)$$

$$M_{n+1}X_n + 2HF = M_{n+1}X_nF_2 + H_2 \quad (3)$$

The extraction of aluminum from the MAX phase material is shown Eq. 1, while Eqs. 2 and 3 show the generation of -OH and –F functional groups respectively [38,39]. The etching conditions can be adjusted to control the distribution of the functional groups, thereby making it possible to customize the application of MXene products. For instance, by reducing the concentration of HF, the reaction presented in Eq. 3 would be constrain leading to a decrease in the proportion of -F functional groups on the synthesized MXene product [40]. Fig. 3 shows a diagram that depicts the MXene production process as captured by Charan et al. [41]. The stacked MAX phase powders are stirred for a specified amount of time at room temperature while aqueous HF acid is present. Consequently, the A layers undergo selective etching, and the metallic bonds holding the MX layers are displaced with weak bonds of surface terminations such as hydroxyl, fluoride, or oxygen on the MXene surface. The number of M layers separating the A layers determines how the MAX phases differ from one another [41].

In order to create novel MXenes with greater control over their surface chemistries, several synthesis methodologies have been developed over the past decade. A mixture of non-aqueous etchants, halogens, fluoride salts, and various acids have been selectively etched to modify the surface properties of MXenes in recent studies [42]. For instance, in 2016, the first nitride-based MXene was produced by the molten salt etching technique [43]. $Ti_4AlN_3$ powder was etched to create the Al layer portion using a molten fluoride salt mixture (59 % KF, 29 % LiF, and 12 % NaF) at 550℃. Tetrabutylammonium hydroxide was then used to delaminate the powder to create monolayers of $Ti_4N_3Tx$ MXene,

MXenes, typically synthesized through wet chemical acidic etching of MAX phases, are utilized in two primary forms: as a stable colloidal suspension containing single or few-layer flakes or as multilayer stacks of MXene sheets. The post-etching processing steps play a critical role in determining the production efficiency and quality of these forms [44]. The schematic illustration of selective etching and sonication of MXenes with hydroxyl and fluorine atoms is presented in Fig. 4. Selective etching technique (shown in Fig. 4) can effectively stabilize MXenes against structural degradation brought on by spontaneous oxidation and

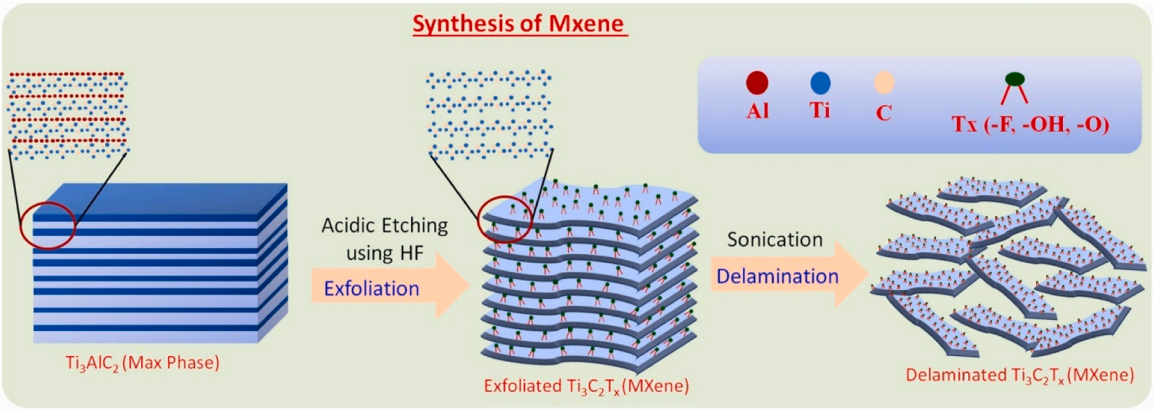



**Fig. 3.** Illustration of the process of MXene synthesis process [41]. Culled with permission from Elsevier.

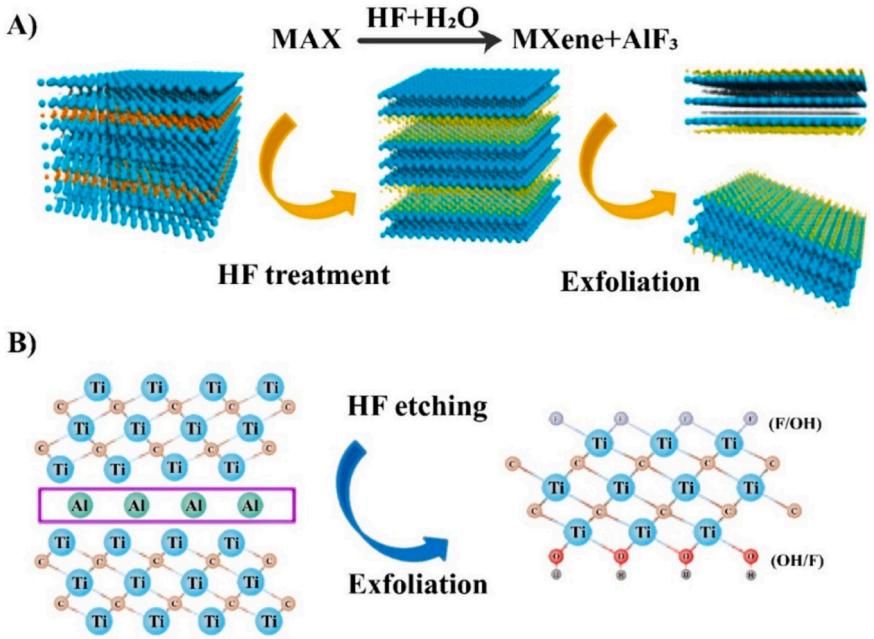



**Fig. 4.** Schematic illustration of selective etching of the MXenes with hydroxyl and fluorine atoms [8]. Culled with permission from Elsevier.

enhance surface characteristics [8].

Fig. 5 provides scanning electron microscopy (SEM) images of MAX, MXene, and colloidal MXene and visual depictions of the etching process.

Fig. 5a presents the analysis of the Scanning electron micrographs showing Ti3AlC2 MXene particles in the form of flakes in the colloidal suspension. In Fig. 5b, the SEM micrographs reveal A synthetic water-dispersible Ti3C2Tx utilizing tin fluoride, SnF2, is shown in Fig. 5. Ti3AlC2 and SnF2 combination is heated, then delamination is achieved by sonication, followed by washing and intercalation with KOH and DMSO, as shown in Fig. 5. Although Fig. 5(b and c) shows the unusual presence of crystalline structures intercalating the layers, the synthesized Ti3C2Tx has the typical accordion structure, indicating that aluminum was successfully etched from the MAX phase. These structures were thought to be SnF2 and AlF3 salts, resulting from the diffusion of SnF2 between the layers during the etching and formation of AlF3. Given the substantial differences in quantity and physical characteristics between colloidal and MXenes, it is crucial to emphasize the merits and drawbacks of each form. Exploring how these two forms can be effectively employed in polymer nanocomposites (NCs) is essential for a comprehensive understanding of their applications [22].

One prominent application of MXenes lies in energy storage systems. MXenes exhibit excellent electrical conductivity and large surface areas, making them promising materials for supercapacitors. MXenes play a vital role in advancing high-performance energy storage devices due to their efficiency in storing and delivering energy [46]. MXenes have found applications in the field of catalysis. By customizing the surface chemistry of MXenes, their catalytic activity can be improved, making them effective catalysts for various chemical reactions. This versatility positions MXenes as catalysts for applications such as water splitting, where they produce hydrogen, a clean and sustainable fuel [47].

The consideration of MXene products for sensors and electronic devices has introduced a range of adjustable electronic properties and sensitivity to environmental changes, rendering them well-suited for sensing applications. MXene-based sensors can detect gases, biomolecules, and environmental pollutants, showcasing their potential in creating advanced and responsive sensing devices [48]. Also, in the field of composites and materials science, MXenes are being explored for reinforcing polymers and enhancing material properties. Integrating MXenes into polymers leads to composite materials exhibiting enhanced mechanical strength, thermal stability, and conductivity [49]. This paves the way for the creation of advanced materials characterized by

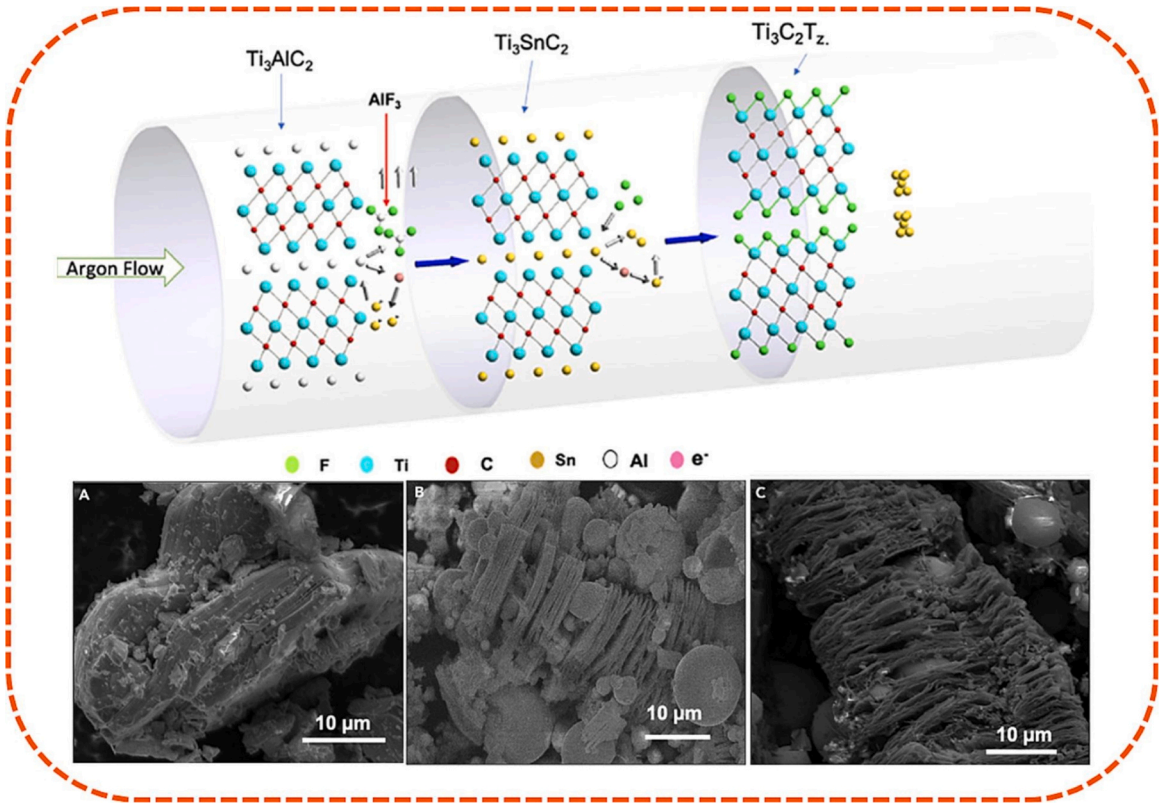



**Fig. 5.** Schematic of the reaction setup used for molten salt etching in a tube furnace under argon flow to minimize the interference of oxygen during etching. FESEM images of (A) Parent $Ti_3AlC_2$ MAX phase, (B) $Ti_3C_2T_x$ before KOH wash (freeze-dried), (C) $Ti_3C_2T_x$ after KOH wash (freeze-dried) [45]. Culled with permission from Elsevier.

improved performance and durability.

## 2. Traditional material design and characterization methods versus MXenes characterization

Traditional material design and characterization methods face several challenges when applied to MXenes, hindering a comprehensive understanding and optimization of these promising materials. One significant limitation lies in the difficulty of capturing the intricate surface chemistry of MXenes. Traditional techniques often fall short of providing detailed insights into the diverse surface terminations and functional groups that critically determine the properties of MXenes [50]. As a result, a clear understanding of MXene surface modifications, which is essential for tailoring their properties, remains elusive.

Determining the thickness of MXene layers poses a challenge for conventional characterization methods. Methods such as X-ray diffraction and transmission electron microscopy may face challenges in accurately measuring the thickness of MXene layers, particularly when dealing with few or single atomic layers. The accurate determination of layer thickness is paramount as it directly influences the electronic and mechanical properties of MXenes [51].

Traditional methods also encounter difficulties in capturing the dynamic behavior of MXenes. Many MXenes exhibit dynamic changes in their surface functional groups under specific environmental conditions [52]. Traditional techniques, which often provide static snapshots, cannot monitor and understand these dynamic transformations. To comprehend the full range of MXene behaviors, there is a need for advanced in situ characterization methods that can track changes in real-time [53].

Typically, the scalability of MXene synthesis is a concern when employing conventional wet chemical etching processes [54]. These processes may be time-consuming or involve harsh conditions and challenging large-scale production. Overcoming this limitation is essential for realizing the full potential of MXenes in practical applications, particularly in industries that demand scalable and cost-effective production methods [55].

In the context of MXene-polymer composites, traditional methods face challenges in probing the molecular-level interactions between MXenes and polymers. Understanding these interactions is crucial for optimizing the performance of composite materials. Traditional techniques may lack the resolution needed to elucidate the detailed nature of the bonding and compatibility between MXenes and polymer matrices [56].

## 3. The role of machine learning in characterization of MXenes

Machine learning (ML) is pivotal in overcoming the limitations associated with traditional material design and characterization methods for MXenes, offering a pathway to accelerate research and development in this field [57,58]. ML algorithms excel in handling complex datasets and can analyze enormous amounts of information, giving insights that may be challenging for conventional methods. In the case of MXenes, machine learning can aid in unraveling intricate surface chemistry by identifying patterns and correlations within experimental and computational data. This makes it possible for researchers to elucidate the relationships between MXene properties and various synthesis parameters, facilitating the design of MXenes with tailored characteristics [51].

ML algorithms are also instrumental in predicting and optimizing MXene properties, especially thickness determination. By training models on diverse datasets that include experimental thickness measurements, computational simulations, and other relevant parameters, machine learning can enhance the accuracy of predicting MXene layer thickness [57]. This addresses a critical limitation of traditional

techniques and allows for the efficient design of MXenes with desired electronic and mechanical properties.

Machine learning supports the exploration of dynamic behaviors in MXenes. ML algorithms can analyze time-dependent data, identifying trends and changes in MXene structures over different conditions [59]. This capability enables researchers to capture and understand the dynamic nature of MXene surface modifications, providing valuable insights into their behavior under varying environmental factors [17]. In terms of scalability and synthesis optimization, machine learning contributes by assisting in the development of predictive models for efficient production processes. By analyzing synthesis conditions and outcomes from various experiments, ML algorithms can suggest optimized parameters for scalable and reproducible MXene synthesis, thereby expediting large-scale production efforts [14,60].

Machine learning also aids in deciphering the intricate interactions between MXenes and polymers in composite materials [61]. Complex molecular features of MXene-polymer interactions can be uncovered by ML algorithms through the use of computational models and experimental data analysis. This understanding is crucial for tailoring composite materials with enhanced mechanical, thermal, and electrical properties. By harnessing the capabilities of ML algorithms, researchers can accelerate the discovery, design, and optimization of MXenes, leading to advancements in energy storage, catalysis, sensing, and materials science.

## 4. Machine learning applications in MXene design, synthesis and characterization

### 4.1. Machine learning methods

Computers can learn and adapt by utilizing large datasets and ML applications to eliminate numerous risks and dead ends in programming. These algorithms possess the ability to identify patterns, extrapolate from training data, and adapt over time. In the realm of risk assessment, diverse ML approaches find application within the literature. The domain within computer science, "machine learning," pursues discerning patterns from data to improve performance across diverse activities [62]. The various methods involved in machine learning operation is presented in Fig. 6.

ML is a potent tool in materials science, with notable applications in the design and synthesis of functional materials, exemplified by MXenes [48]. Some key areas where ML methods are utilized in MXene characterization include:

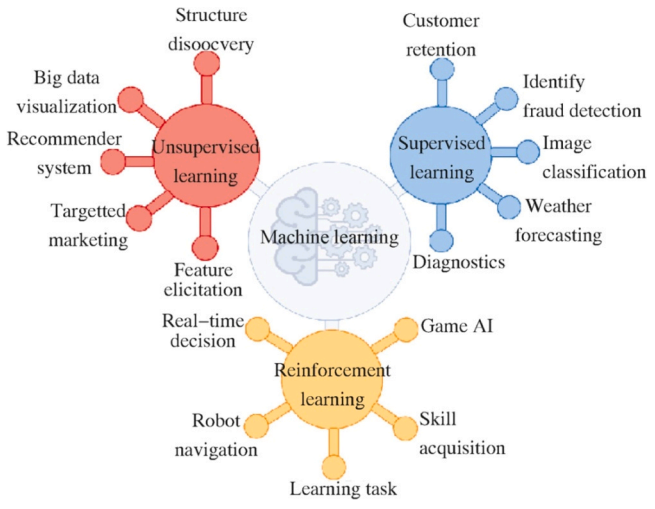



**Fig. 6.** Categorization of Machine Learning Algorithms showing the supervised learning, unsupervised learning, and reinforcement learning [63]. Culled with permission from Elsevier.

i. Materials Property Prediction: ML models can predict various material properties of MXenes, such as electronic band structures, mechanical properties, and thermal conductivity and these predictions aid researchers in identifying MXenes with desirable characteristics for specific applications [57].
ii. Accelerated Discovery: ML algorithms enable the rapid screening of potential MXene candidates from a vast chemical space which also accelerates the materials discovery process by suggesting compositions and structures that are likely to exhibit desired properties [57].
iii. Structure-Property Relationships: ML helps to establish complex relationships between the structural features of MXenes and their properties to facilitates the targeted design of MXenes with optimized performance for specific applications [64].
iv. Synthesis Optimization: ML algorithms can analyze data from experimental processes to optimize conditions for MXene fabrication. This includes predicting the most favorable synthesis parameters, such as temperature, precursor ratios, and reaction times [65].
v. Identifying Novel MXene Compositions: ML algorithms are employed for analyzing existing MXene databases and literature to identify patterns and propose novel compositions or structures that have not been explored [66].
vi. Property-Driven Material Design: ML algorithms facilitate a data-driven approach to material design by considering multiple properties simultaneously. This helps researchers to optimize MXene compositions not only for a single property but for a combination of properties tailored for specific applications [67].
vii. Fault Detection and Quality Control: ML algorithms can be applied to analyze experimental data to detect any anomalies or deviations in the synthesis process for quality control that ensures the reproducibility of MXene materials [67].
viii. Active Learning for Experimental Design: ML-driven active learning approaches can guide experimental design by selecting the most informative experiments for reducing the number of experiments needed to characterize and understand MXene properties [68].

Machine learning methods have been applied in so many fields to help speed up the process of data acquisition by utilizing current experimental and theoretical data to predict the different materials properties. For MXenes, ML methods can help through every process, from materials design, synthesis, and identifying new MXene compositions, enabling quick identification of potential candidates and optimum processing conditions for obtaining desired material properties.

### 4.2. Prediction of MXene surface functionalization, composition, and morphology using machine learning models

ML models are crucial in predicting MXene surface functionalization, composition, and morphology by offering valuable insights and accelerating the materials discovery process [69]. ML models can copy and adapt patterns from existing data on MXenes and their functionalization processes [20]. By analyzing experimental parameters (such as reaction time, temperature, precursor concentrations) and experimental outcomes, ML models can predict the likely functional groups attached to the MXene surface. This is particularly useful for tailoring surface properties for specific applications such as catalysis or sensing. A range of experimental parameters can be analyzed to predict the optimal conditions for achieving desired surface modifications efficiently [69]. Machine learning models predict the composition of MXenes based on various input features, including precursor materials, reaction conditions, and synthesis methods [66]. This aids researchers in identifying suitable compositions for targeted applications, taking into account the desired electronic, optical, or mechanical properties. For MXenes with multiple components or layers, ML models can predict the composition

of each layer, and this helps to understand the complex structure and its impact on material properties.

In the prediction of morphological features, ML models can analyze data on synthesis methods, precursor properties, and experimental conditions to predict MXene morphology, including layer thickness, lateral size, and overall structure. This is essential for tailoring MXene morphology for specific applications, such as energy storage or catalysis. Also, ML-driven optimization suggest synthesis conditions that yield desired morphological characteristics by learning from a dataset of experimental outcomes to propose conditions that lead to the formation of MXenes with specific morphologies [70].

### 4.3. Applications of data-driven approaches and density functional theory (DFT) models

Electronic structure methods encounter challenges due to their unfavorable computational scaling. Conducting large-scale calculations involving more than a few thousand atoms demands substantial computational resources and time investment. Data-driven workflows present a solution by providing accelerations through supplementation or substitution of conventional density functional theory (DFT) calculations [71]. In the last thirty years, there has been a significant increase in the accumulation of extensive theoretical and experimental data spanning various knowledge domains. In computational materials science, this large quantity of data is credited mainly to the success of density functional theory (DFT) and the rapid advancements in computational capabilities [72]. Concurrently, progress in instrumentation and electronics has empowered experiments to generate significant amounts of data. This lays the foundation for the development of innovative tools capable of extracting knowledge from theoretical and experimental database [73]. The domain of statistical learning is the key factor that drives the various ML techniques in current research and development. The DFT is based on two theorems expounded in [74], which characterize the structure and properties of organic materials such as MXenes. These theorems demonstrate that: (i) in a system containing MMM electrons, the external potential V(r) acting on the electrons is uniquely determined by the electronic density m(r); and (ii) the ground-state energy $E_G$[m] attains its minimum value for the exact electronic density [75].

These theorems can be mathematically stated as Eq. 4.

$$EG = \mathrm{EG}[(m(\mathbf{r})] \tag{4}$$

The external potential is considered as a functional of the ground-state density as expressed in Eq. 5.

$$\mathrm{EG[m]} = \mathrm{T_s[m]} + \mathrm{U_H[m]}\ \mathrm{V_{ext}[m]} + \mathrm{EG_{xc}[m]} \tag{5}$$

Given that the forms of some of the functionals are already known, where $U_H$ denotes the Hartree potential, $T_s$ is the Kohn-Sham kinetic energy, and $V_{ext}$ is recognized as an external potential. The Kohn-Sham kinetic energy for the non-interacting reference system is expressed in Eq. 6 [76].

$$\mathrm{Ts[m]} = \sum_i \left\langle \phi_i \middle| -\frac{1}{2}\nabla^2 \middle| \phi_i \right\rangle \tag{6}$$

Eqs. 7 and 8 can be resolved to derive the well-known Kohn-Sham (KS) Eq. 9.

$$\left( -\frac{1}{2}\nabla^2 + v_{eff}(\boldsymbol{r}) \right)\phi_j(\boldsymbol{r}) = \epsilon_j \phi_j(\boldsymbol{r}) \tag{7}$$

$$v_{eff} = v_{ext}(\boldsymbol{r}) + \int \frac{m(\boldsymbol{r}')}{|\boldsymbol{r} - \boldsymbol{r}'|} d\boldsymbol{r}' + v_{xc} \quad (\boldsymbol{r}) \tag{8}$$

$$m(\boldsymbol{r}) = \sum_j |\phi_j(\boldsymbol{r})|^2 \tag{9}$$

Where $f_j$ represent the Lagrange multipliers commonly understood as the energy levels of the Kohn–Sham orbitals, this set of equations outlines a self-consistent cycle: one starts with a tentative density m(r), includes a functional form of $v_{xc}$, and constructs the effective potential $v_{eff}$, the electronic density is then determined from the set of $f_j$ eigenvector values, and the process iterates until convergence criteria, typically based on the system's total energy, are achieved.

Abraham et al. [77] established a ML/DFT-based workflow using supervised machine learning models to evaluate the hydrogen evolution reaction (HER) performance of 4500 $MM'XT_2$-type MXenes. With a low predictive mean absolute error (MAE) of 0.358 eV, the gradient boosting regressor (GBR) processed with recursive feature elimination (RFE), hyperparameter optimization (HO), and the leave-one-out (LOO) approach is the most desirable machine learning model. It predicts the Gibbs free energy of hydrogen adsorption ($\Delta G_H$) accurately and quickly. The H atoms absorbed directly on top of the outermost metal-atom layer of the MM'XT2-type MXenes (site 1) with Nb, Mo, and Cr metals with O functionalization are found to be extremely stable and active for catalysis, outperforming their commercially available platinum-based counterparts, according to these model predictions.

In recent study, Haider et al. [78] used random forest (RF) and convolutional neural network models (CNN) to predict the heat of formation of several MXene materials. The neural network model predicts the heat of formation using 12 different MXenes characteristics, with a mean absolute error (MAE) of 0.18 eV on training data and 0.21 eV on testing data. In this study, it was found that the CNN model outperformed the RF models.

When combined with first-principles ab-initio computations, ML marks a paradigm change in materials research. Understanding the basic behavior of materials depends much on ab-initio techniques such as DFT, which solves quantum mechanical equations to forecast material properties with great accuracy [79]. It is rather important to know various parameters effect on the thermodynamic favorability and stability of MXenes in diverse applications. However, these methods are computationally difficult and time-consuming particularly for large or complex systems.

This section recognizes the high impact of the application of ML methods in transforming MXenes research serving as high throughput substitutes for intensive and laborious first principles methods. These models can predict important MXene properties and structures such as surfaces, electronic band structures, elemental compositions, structural uniformity, layer thickness and morphology by mining existing experimental and DFT derived datasets. When DFT theorems are embedded into data-driven processes, self-consistent physics based models are developed that scales to thousands of candidates while maintaining the quantum mechanical accuracy. The push to replace or augment the DFT takes advantage of both methods' advantages, drastically reducing the search space for new materials to training quick, scalable algorithms employing physics-based descriptors.

### 4.4. Determination of the electronic band structures, mechanical strength, and catalytic activity using ML

Computational methods efficiently analyze experimental data, translating it into valuable information. This computational data analysis mitigates the risk of artificial misinterpretation and significantly improves the accuracy of analysis and description [80]. The application of ML in material science can be categorized into three primary domains: prediction of material properties, designing and discovering new materials, and achieving various other objectives.

In predicting material properties, ML techniques operate at both macroscopic and microscopic levels, often employing regression analysis methods [81]. ML approaches construct probabilistic models to sift through potential combinations of structures and compositions to discover and design new materials. Post-sifting, the algorithm selects

materials with the desired qualities and performance from the diverse combinations. Subsequently, the chosen material undergoes validation through DFT-based methods. Beyond prediction and discovery, ML finds utility in other material science objectives, such as recognizing microstructural materials and optimizing processing methods [82].

Atomic catalysts (AC), at the forefront of electrochemistry, have gained significant consideration currently owing to their exceptional electroactivity with diverse applications in energy conversion and storage [83]. Presently, many support materials and flexible choices for anchoring metal elements characterize the landscape of atomic catalysts. The permutations resulting from the combinations between support and elements across the periodic table offer extensive possibilities. However, the existing research on atomic catalysts is predominantly conducted on a case-by-case basis, incurring substantial costs and lacking a clear direction to pinpoint the most promising ACs with superior electroactivity and stability [84]. In addressing this challenge, ML emerges as a potent tool, providing an efficient and accurate strategy for screening the desired electrocatalysts tailored for various electrochemical reactions. ML algorithms have found application across a different of material classes, including polymers, metals and alloys, 2D materials, ceramics and composites, organic-inorganic hybrids, and multi-component hetero-anionic compounds [62]. These algorithms excel in uncovering potential non-linear relationships involving multiple variables. Significant achievements in the application of ML for forecasting material properties encompass the estimation of energetics, phase stability, cation/anion arrangement, defect energetics, bandgaps, melting and glass transition temperatures, mechanical and elastic properties, thermal conductivity, dielectric properties, crystallization tendency, catalytic activity, and resistance to radiation damage.

Zhou et al. [85] predicted the electronic band structures of 2D materials using a neural network trained on DFT-calculated data. This method has improved the efficiency of the discovery process by making it easier to identify materials with optimal band gaps and carrier mobility for electrical applications. By applying Gaussian Process Regression (GPR) to MXene data, Li et al. [86] also made substantial progress in their selection for catalysis and energy storage applications by using descriptors such as electronegativity and atomic radii to predict work functions and other important electronic features.

Applying predictive modeling techniques to DFT computations has hastened the innovation of advanced materials, drastically reducing the search space for experiments. Also, the accurate prediction of mechanical properties, especially in the context of concrete design codes, has presented a challenge. Researchers are actively working on precise models to forecast mechanical strength, particularly by introducing novel concrete mixtures and applications [87].

## 5. Design and development of novel MXenes

### 5.1. Application of ML-driven exploration for design of new MXene phases

ML encompasses various techniques such as regression, classification, and clustering; and these approaches share a commonality in their utilization on pre-existing datasets, which should be sufficiently large to encapsulate pertinent information [88]. To render these datasets applicable, they are represented through a set of features or descriptors, either derived directly from the datasets or acquired through data preprocessing. Machine learning methods are broadly categorized into supervised and unsupervised learning algorithms. In supervised learning, the ML algorithm is provided not only with features but also with the target quantity, which is subsequently employed to train the model [89].

In materials science, it is common practice to adjust physical models based on experimental and theoretical data by varying the model parameters to minimize errors in predicting properties [90]. However, it is imperative to quantify and handle uncertainty systematically to validate the model.

Calculations within electronic structure theory allow for the comprehension of matter at the quantum level, serving as a valuable complement to experimental studies in both material science and chemistry. These calculations play a pivotal role in addressing critical scientific and technological challenges. The emergence of modern, high-performance computational resources has facilitated extensive electronic structure simulations [91]. However, the escalating demand for precise first-principles data renders even the most efficient simulation codes impractical.

Conversely, the adoption of data-driven machine-learning (ML) methods has experienced rapid growth across various research domains. These methods are increasingly significant as they are employed to expedite, replace, or enhance traditional electronic structure theory techniques. Density functional theory (DFT) frequently serves as the computational backbone in electronic structure workflows. While DFT offers a favorable trade-off between computational cost and accuracy, substantial speed improvements can be realized when it is integrated with ML [92].

### 5.2. Use of genetic algorithms, evolutionary algorithms, and Bayesian optimization for material discovery

Genetic algorithms (GAs) have emerged as powerful tools in the field of material discovery, offering a systematic and efficient approach to exploring vast design spaces and identifying novel materials with desired properties [93]. The use of genetic algorithms in material science leverages principles inspired by natural evolution and genetic mechanisms to optimize and discover materials that meet specific criteria [94]. Genetic algorithms (GAs) are metaheuristic optimization techniques inspired by Darwin's theory of evolution. These algorithms evolve into a population of candidate solutions through the iterative application of crossover, mutation, and selection operations. By carefully designing operators and optimizing parameters, GAs can exhibit remarkable robustness in solving complex optimization problems [95]. This robustness stems from their ability to explore and generate solutions that might be difficult to predict in advance. However, GAs often requires numerous function evaluations, as typical offspring may not inherently represent "fit" solutions. In modern machine learning (ML), GAs have proven capable of modeling complex functions in high-dimensional feature spaces while effectively mitigating the risk of overfitting [96].

### 5.3. Concepts of genetic algorithms

The concept of genetic algorithm is based on several principles stated as follows:

i. Inspiration from Natural Evolution: Genetic algorithms draw inspiration from the principles of natural selection and evolution. In nature, species evolve over time through the inheritance, mutation, and selection of genetic traits. Similarly, in genetic algorithms, a population of potential solutions (individuals) evolves over generations through genetic operators such as mutation, crossover (recombination), and selection [97].
ii. Representation of Materials: Genetic algorithm represents materials as sets of parameters or attributes that define their properties. These parameters could include composition, crystal structure, electronic structure, or other relevant characteristics depending on the specific application [98].
iii. Objective Function: The optimization process in genetic algorithms is guided by an objective function. This function quantifies how well a particular set of parameters fulfills the desired material properties [97]. The goal is to find the parameters that maximize or minimize the objective function, depending on the specific optimization problem.

Genetic algorithms (GAs) frequently rely on semi-empirical potentials to describe the potential energy surface (PES) in materials science and applications. The utilization of more accurate methods, such as density functional theory (DFT), to represent the PES has been limited by computational costs. Recognizing the heightened computational demands associated with directly exploring the PES using DFT, studies have frequently faced limitations in terms of scale, although these approaches have proven successful in various investigations [82].

The ML-accelerated Genetic Algorithm (MLaGA) integrates a two-tier energy evaluation process: one tier utilizes machine learning (ML) models to predict fitness, while the other relies on an energy calculator to determine actual fitness [99]. Within this framework, a nested GA operates on a surrogate model generated by ML, enabling high-throughput screening based solely on predicted fitness in the "master" GA [98]. The nested GA leverages the current population to perform additional search iterations, where evaluation and selection are guided exclusively by the ML-based representation of the Potential Energy Surface (PES) [98]. This method allows significant exploration of the PES without incurring the computational cost of extensive energy evaluations.

However, traditional convergence criteria used in standard GAs are less applicable to MLaGA [100]. In MLaGA, convergence is achieved when the ML model prevents new candidate evaluations, halting the search. The GA can operate with a pool of candidates or a generational population. In the generational population approach, an ML model is trained and applied to evaluate an entire generation of candidates. Combining MLaGA with the nested GA approach expands the candidate pool compared to traditional GAs, but many candidates are filtered out before reaching the computationally expensive energy evaluation stage [101].

This nested search strategy enables efficient identification of the full convex hull of minima, typically requiring an average of 1200 candidates. Further optimization, such as adjusting acceptance criteria with methods like Tournament acceptance, can enhance efficiency, reducing the number of necessary energy minimizations to fewer than 600.

The MLaGA can also operate with a pool-based population, wherein the surrogate model is retrained for each new data point generated by electronic structure calculations [101]. However, this approach progresses serially, potentially increasing computation time due to the lack of parallelizability in electronic structure calculations. This method requires around 310 energy minimizations to explore the convex hull.

Training a new model for each energy calculation makes it possible to estimate and incorporate model prediction uncertainty, as detailed in the "GP regression model" section of the Methods. When the cumulative distribution function is employed as the fitness measure, the pool-based MLaGA identifies the convex hull of stable minima with approximately 280 energy calculations [98].

Evolutionary algorithms (EAs) are a class of soft computing techniques designed as problem-independent search methods applicable to a wide range of optimization challenges, including drug design and discovery [102]. These population-based metaheuristic optimization techniques draw inspiration from biological evolution, utilizing principles such as reproduction, mutation, recombination, and selection. EAs function as randomized, stochastic approaches, simulating the evolutionary pressures of natural selection to promote the survival and propagation of high-fitness individuals [103].

Guided by the principle of "survival of the fittest," EAs begin with a population of randomly generated solution candidates that evolve over successive generations. High-fitness individuals (parents) from each generation undergo crossover to produce offspring, experience mutations and are selected for the next generation based on defined survival criteria [104].

### 5.4. Components of evolutionary algorithms

Given the vast search space inherent in de novo drug design, evolutionary algorithms prove beneficial in identifying optimal solutions, specifically novel drugs. An advantage lies in their ability to operate without requiring a labeled training set, distinguishing them from generative deep learning methods. Evolutionary algorithms are particularly promising for addressing the synthesizability problem in de novo drug design [105]. Additionally, they exhibit the capacity to optimize multiple, sometimes conflicting, objectives, a crucial aspect in drug design where potential candidates need to be bioactive, synthesizable, and possess other drug-like characteristics [106]. Evolutionary algorithms encompass the following key components:

i. Representation: This involves genotype representation and genotype-phenotype mapping.
ii. Parent Selection: The process of choosing individuals for crossover based on their fitness.
iii. Crossover Operators: Mechanisms for forming new individuals by combining parent individuals.
iv. Mutation Operators: Introducing random changes to parts of an individual's genome.
v. Termination Condition: Specifies when the algorithm should cease its iterations.

### 5.5. Bayesian optimization

Bayesian optimization (BO) has emerged as a powerful and efficient method for material discovery, offering a systematic approach to navigating complex and high-dimensional parameter spaces [107]. In materials science, where discovering novel materials with specific properties poses a significant challenge, Bayesian optimization offers an intelligent framework to steer experiments and simulations. Fundamentally, Bayesian optimization integrates probabilistic modeling with optimization to effectively explore the optimal set of parameters [108]. It utilizes a probabilistic surrogate model, commonly a Gaussian process (GP), to capture the inherent behavior of the objective function [109]. This surrogate model provides predictions of the objective function and estimates of uncertainty, which is crucial for making informed decisions about where to explore next in the parameter space. One significant advantage of Bayesian optimization is its ability to balance exploration and exploitation [110]. In the context of material discovery, this means efficiently exploring the parameter space to discover promising regions while also exploiting the current knowledge to refine the search in areas likely to contain optimal materials. This balance is particularly valuable in cases where experiments or simulations are costly and time-consuming, as it helps prioritize the most informative evaluations. The Bayesian optimization process begins with initial experiments or simulations to establish the surrogate model. As the optimization progresses, the surrogate model is updated iteratively with new observations, continuously refining its predictions [111]. The acquisition function, a crucial element in Bayesian optimization, directs the choice of the next set of parameters to assess. Expected Improvement (EI) and Probability of Improvement (PI) are two often utilized acquisition functions, both quantifying the potential gain in the objective function or the likelihood of discovering a superior solution. Bayesian optimization finds applications in the discovery of novel MXenes. For example, it can be employed to optimize the synthesis conditions for a new material by efficiently exploring the space of parameters such as temperature, pressure, and precursor concentrations [112]. Additionally, it can guide the search for optimal material properties, such as electronic bandgap or mechanical strength, by tuning the composition or structure of the material. The use of Bayesian optimization in material discovery aligns with the broader paradigm of data-driven and machine learning-driven approaches in materials science It allows researchers to navigate the vast and complex design spaces more intelligently, accelerating the pace of discovery and facilitating the identification of materials with desirable properties for specific applications [94]. Integrating Bayesian optimization with advanced experimental

techniques and computational methods offers transformative potential for material science, significantly accelerating the discovery and development of innovative materials. Bayesian optimization predicts the relationship between explanatory variables (e.g., synthetic conditions like temperature and pressure) and objective variables (e.g., transmittance and electrical resistance) based on acquired data [113]. By systematically exploring the global optimum, it leverages the prediction curve and confidence interval generated from the data.

The Bayesian optimization process can be summarized as follows [113]:

1. **Initial Data Collection:** Obtain initial data points.
2. **Prediction Model Development:** Use collected data to calculate a prediction curve and confidence interval (standard deviation) for the objective variable.
3. **Candidate Optimization:** Apply the prediction model to prioritize synthetic conditions using an acquisition function, identifying a candidate global optimum.
4. **Data Refinement:** Collect additional data based on the candidate conditions from step 3 and return to step 2.

This iterative process continues until the optimal synthesis conditions are identified.

In a recent work, Mhadeshwar et al.[114] used DFT-predicted elastic modulus datasets to estimate the elastic modulus of novel boride-based M2AX phase materials utilizing the XGBoost (XGB) regressor model and Bayesian optimization. The elastic moduli of 223 M2AX phase materials (carbides and nitrides) were predicted using an ensemble of gradient boosted machine learning models. In order to find the most desirable characteristics and maximize the model-predicted elastic modulus, inverse modeling was employed using Bayesian optimization. In order to uncover potentially novel materials, model predictions for 1035 M2AX materials were generated and compared to the most desirable attributes. The high elastic moduli (347–372 GPa) of Ta2PB, Nb2PB, and V2PB were found to be comparable to those of their carbide counterparts (357–374 GPa). These findings further suggest that borides may be a feasible tertiary element for M2AX phases.

Within the Bayesian optimization framework, the prediction model for the objective variable—representing a property value—is typically developed using Gaussian process regression or similar methods [115]. The property value under a specific experimental condition xxx is expressed as a probability distribution, often modeled as a normal distribution p(y|x. The prediction curve corresponds to the mean of this distribution, while the standard deviation (variance) reflects the uncertainty in the prediction [116].

This section focused on describing the impact of data-driven and evolutionary optimization strategies in transforming the discovery of new MXene phases. In order to propose viable new compositions, its emphases and describes the role of supervised and unsupervised ML methods in mining vast amounts of datasets, quantify uncertainty and embed physics-based descriptors, the use of nested ML accelerate GAs (MLaGA) in selecting candidates prior to expensive energy evaluations. Bayesian Optimization and XGBoost are also effective techniques for exploring the large, high dimensional compositional materials landscape significantly reducing the computational and experimental load associated with MXene design.

## 6. Commercialization of MXene products

Commercial utilization of MXenes in applications including energy storage, catalysis, and electronics has already begun [11]. Some specific MXene products will be discussed in the following section.

### 6.1. $Ti_3C_2$ MXene for energy storage

Titanium carbide ($Ti_3C_2$) MXene has demonstrated remarkable performance in energy storage applications, particularly in supercapacitors (SCs), garnering significant research attention [50]. Its large surface area, excellent electrical conductivity, and high ion-holding capacity make it a promising candidate for energy storage devices. $Ti_3C_2Tx$ can be employed directly as an active material or serve various roles, such as an electrocatalytic material, support, conducting agent, or buffer layer in composite electrode construction [117,118]. In direct applications, $Ti_3C_2Tx$ is primarily utilized in supercapacitors (SCs) and sodium-ion batteries (SIBs). The specific capacitance of highly exfoliated MXenes for SCs is influenced by their surface area and the chemical nature of their surface terminations. In contrast, the performance of bulk MXenes in battery electrodes—such as rate capability, irreversible capacity, and average voltage—is determined by factors like crystalline order, phase purity, topology, and termination type. In order to optimize the critical operating parameters for the photocatalysis water splitting application of Ti3C2 MXenes, Karimi et al. [119] developed data-driven machine learning models. To supplement the inadequate experimental data, virtual datasets were generated using a Gaussian mixture model (GMM). The accuracy of an ANN model in forecasting critical operational parameters such the concentration of photocatalyst, pH, temperature, solar irradiation, and ethanol concentration was greatly increased by this augmentation strategy. In the end, the improved model offered an efficient data-driven framework to hasten the design and implementation of effective $Ti_3C_2$ MXenes-based hydrogen production systems.

### 6.2. $Ti_3C_2T_x$ MXene for electrode-based supercapacitor applications

Supercapacitors operate through two primary charge storage mechanisms: electrical double-layer capacitors (EDLCs) and pseudo-capacitors. In EDLCs, an electrostatic double layer forms as charges accumulate at the electrode/electrolyte interface. This process stores energy through a non-Faradaic mechanism, meaning it does not involve electron transfer or redox reactions [118]. Conversely, pseudo-capacitors rely on Faradaic redox reactions, where electron transfer occurs, largely independent of the electrode's surface area. In this case, electrolyte ions migrate through the electrode into a conducting bulk phase during the redox process [120]. Unlike Faradaic processes, non-Faradaic mechanisms retain charges within the electrode without them exiting.

The charge storage mechanism of EDLCs is characterized by the shape of the cyclic voltammogram (CV) curve, which reflects the atomic composition of the electrodes. $Ti_3C_2Tx$ MXenes, with their rich functional groups and layered structure, facilitate charge accumulation, making them highly effective for energy storage [121]. In MXenes, redox reactions and energy storage occur within the active functional groups and at the interfaces between their layers.

To achieve high energy density and stability in supercapacitor electrode materials, researchers are exploring MXene-based and hybrid electrode architectures. However, several persistent challenges continue to affect the energy storage efficiency of MXene-based electrodes, necessitating further research and innovative solutions [122].

### 6.3. $Mo_2TiC_2T_x$ MXene for electrocatalysis applications

Molybdenum titanium carbide ($Mo_2TiC_2Tx$) MXene has demonstrated outstanding electrocatalytic activity for key reactions such as the hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR), owing to its unique electronic structure and surface chemistry [123]. This makes it an efficient catalyst for clean energy applications, especially in addressing current energy and environmental challenges through the development of hydrogen energy. HER is a critical process for hydrogen production via water splitting, a cornerstone of the envisioned hydrogen economy. Developing HER catalysts with exceptional conductivity, stability, and selectivity is essential for improving efficiency by lowering the overpotential required for the reaction.

The Gibbs free energy of hydrogen adsorption ($\Delta G_H$) is a key theoretical descriptor of HER activity, calculated through density functional theory (DFT) computations. Optimal HER activity is achieved when $\Delta G_H$ is near thermoneutral [124]. Recently, MXene-based HER electrocatalysts have garnered significant attention, supported by extensive theoretical and experimental research. Structural engineering, including termination modification, metal-atom doping, nanostructure creation, and hybridization, has been employed to optimize MXenes for HER. As electrocatalysts, MXenes and MXene-based composites are emerging as potential alternatives to Pt-based catalysts [125].

One effective strategy for enhancing the HER activity of MXenes involves nanostructure engineering, such as creating nanoribbons and nanodots. These nanostructures exhibit unique electrical properties, fast electrochemical reaction kinetics, and abundant active sites, making them highly promising HER electrocatalysts. Nanostructuring not only expands the applicability of MXenes but also facilitates the assembly of active components [8]. According to DFT simulations, the edges of MXene nanoribbons containing metal and C (or N) atoms can effectively capture hydrogen species, serving as active sites for rapid hydrogen generation.

Various synthetic techniques, including ball milling, shaking treatment, and hydrothermal treatment, have been developed to produce MXene nanoribbons and nanodots [126]. These nanostructures directly influence HER activity by affecting the catalytic mechanism, charge transfer, and active sites. MXene nanostructures, ranging from 1D to 3D architectures, show great potential as HER electrocatalysts, offering an exciting avenue for advancing clean energy technologies [127].

### 6.4. $Nb_2CTx$ MXene for electromagnetic interference shielding

Niobium carbide ($Nb_2CT_x$) MXene has exhibited exceptional electromagnetic interference (EMI) shielding effectiveness due to its high electrical conductivity and flexibility [128]. This makes it a promising material for shielding applications in electronic devices and communication systems, particularly because of its excellent thermal conductivity. Notably, 2D MXenes with varying compositions display a wide range of electrical conductivities, from 5 S/cm to over 20,000 S/cm. Their superior electrical conductivity enables MXenes to offer advanced EMI shielding capabilities that outperform traditional metal foils and synthetic materials [129].

MXenes have emerged as leading materials for EMI shielding, primarily due to their unique properties and innovative design features. Unlike conventional shielding materials, MXene films consist of a multilayered laminate architecture composed of 2D MXene sheets. This structure enhances the absorption of incident electromagnetic waves (EMWs) within the shield. A multilayered MXene film achieves efficient EMI shielding with minimal thickness, as each layer contributes positively to attenuating the energy of EMWs.

Moreover, MXene structures can incorporate external inclusions, such as dielectric domains or pores, which promote multiple internal reflections at the interfaces. These reflections further reduce the energy of EMWs, thereby enhancing shielding performance. The surface chemistry of MXenes also plays a crucial role in improving EMW absorption. Polarization losses, particularly dipolar or orientational polarization, dominate in the gigahertz (GHz) frequency range. Negatively charged surface terminations in MXene layers create dipoles, contributing to enhanced EMW attenuation [130].

This combination of high conductivity, multilayered architecture, and surface chemistry positions MXenes as an innovative and efficient solution for modern EMI shielding challenges.

### 6.5. $V_2CT_x$ MXene for water purification

MXene-based nanomaterials have shown significant potential as adsorbents for reducing wastewater contamination [131]. Their intriguing physicochemical properties—such as high surface area, hydrophilicity, strong adsorption capacity, electron density, abundant adsorption sites, efficient ion exchange, and activated metallic hydroxide (OH) sites—make them effective in this role. Additionally, MXenes' excellent redox reactivity allows them to serve as versatile catalysts for pollutant removal through electrocatalysis and photocatalysis. Their ease of synthesis further enhances their applicability for routine environmental remediation [67].

Vanadium carbide ($V_2CT_x$) MXene, in particular, has demonstrated remarkable adsorption properties, especially for the removal of heavy metal ions and organic pollutants from water. Its high surface area and tunable surface chemistry make it an efficient material for water purification [132].

#### 6.5.1. Lead adsorption

Lead is one of the most hazardous pollutants, frequently released into the environment through industrial activities such as mining, pigment manufacturing, fertilizer production, battery manufacturing, and metal plating [133]. MXenes have proven to be highly effective adsorbents with notable lead adsorption capacities, making them useful in a wide range of applications.

When chemically exfoliated using an alkali solution, MXenes can form 2D alk-MXene structures (e.g., $Ti_3C_2(OH/ONa)_xF_{2-x}$), which exhibit promising lead adsorption performance. In one study, a 2D alk-MXene adsorbent achieved adsorption equilibrium within two minutes, with a capacity of 140.10 mg/g [134]. Another method involved preparing MXene from $Ti_3AlC_2$ using hydrofluoric acid and combining it with alginate powder to fill interlayer gaps. This MXene/alginate composite achieved an adsorption capacity of 382.70 mg/g within 15 min [135].

In addition to lead, MXenes have also demonstrated excellent adsorption capacities for other heavy metals, such as chromium and copper. For example, $Ti_2C_2T_x$ MXene nanosheets with oxygenated functional groups have been effectively utilized for copper ion adsorption [46].

These studies underscore the versatility and efficiency of MXenes in environmental applications, particularly for heavy metal removal, positioning them as advanced materials for water purification technologies.

### 6.6. $Ti_2CTx$ MXene for flexible electronics

Titanium carbide ($Ti_2CT_x$) MXene has emerged as a key material for flexible and transparent conductive films, enabling applications in flexible electronics such as displays, sensors, and wearable devices [136]. Its excellent mechanical flexibility, high electrical conductivity, and optical transparency make it a promising candidate for next-generation electronic devices [117]. Wearable technology, in particular, has garnered significant attention as a cutting-edge platform for applications in robotics, health monitoring, motion detection, and prosthetics. These technologies demand exceptional mechanical compliance and unparalleled sensitivity. Flexible electronics designed for wearable devices must conform to complex structures and maintain reliable electrical performance under cyclic strain conditions caused by daily movements—capabilities that exceed those of conventional silicon-based rigid electronics [49]. By addressing these challenges, $Ti_2CT_x$ MXene is advancing the development of innovative, high-performance wearable technologies, paving the way for a new era of interactive and adaptable electronic systems.

It is impossible to overstate the significance of ML-informed models for MXene design, synthesis, and property assessment. This section shows how different data driven models were used for various MXenee materials to help make easy and informed decisions on the commercialization of the MXenes in different applications. Ranging from water purification to help determine the optimal physicochemical properties to redox reactivity allows them to serve as versatile catalysts for pollutant removal through electrocatalysis and photocatalysis. Data-driven models have been extremely helpful in characterizing various

MXene commercial products and in providing quantitative and qualitative data to make informed decisions about the material selection of industrial products in a variety of applications

## 7. Production process of MXenes materials

Much work has been done in the last 10 years to provide a variety of pathways for MXenes preparation using less energy and cost-efficient techniques [137]. When creating MAX phase materials, consideration for green chemistry and clean production should grow steadily. Until yet, the most common methods for generating MXenes from the MAX phase have been water-free etching, electrochemical etching, alkali treatment, and fluoride etching approaches [138].

### 7.1. Fluoride etching

There are two common processes involved in the manufacture of MXenes by fluoride etching. Direct etching with strong Hydrofluoric acid (HF) is one way. MXenes having multilayer structures are etched at room temperature while being constantly stirred, and then they are exfoliated using a sonicator in a mixture of methanol and isopropyl alcohol. The other method involves in situ production of MXene by a reaction between HCl and fluorides to generate a layered structure that is similar to an accordion, according to SEM analysis [139].The effective application of etching with HF or other fluorinated solutions in the synthesis of MXenes has led to the standardization of MXene preparation techniques. However, there are a few issues with this approach. Initially, the strong reactivity of $A_l$ atoms in MAX-phase precursors with F− hindered the synthesis and performance of MXenes. Secondly, the use of fluorinated solutions raises safety concerns and environmental issues [140]. It is not good to end with a problem without mentioning efforts put in place to address them which shall be treated in the succeeding sections.

### 7.2. Alkali etching

Alkali etching is a pivotal process in the realm of MXenes, offering a means to finely tune their properties for myriad applications. This technique involves immersing MXene materials in solutions containing alkali metal compounds, like lithium hydroxide (LiOH), sodium hydroxide (NaOH), or potassium hydroxide (KOH). Through controlled reactions, alkali ions selectively target specific layers or functional groups within the MXene structure, enabling their removal or modification [141]. This process not only alters surface chemistry but also influences interlayer spacing and electronic characteristics. By meticulously adjusting parameters such as solution concentration, temperature, and etching duration, researchers can precisely tailor MXene properties to meet the demands of diverse applications. Post-etching treatments, such as washing and annealing, further refine the material's structure and remove residual etchants [142]. Alkali etching in MXenes thus serves as a versatile tool for surface functionalization, layer exfoliation, and structural optimization, unlocking a wealth of possibilities across fields like energy storage, catalysis, and sensor technology [51].

### 7.3. Electrochemical etching

The basis for chemical etching is the differential in reactivity between M-Al and M-C bonds and direct charge transfer involved in the process is referred to as electrochemical etching. It suggested that in order to produce MXenes without overloading, etching settings needed to be properly adjusted [143]. The variety of etching methods and possible MXene compositions has been expanded via electrochemical etching. There has been a report on thermally assisted electrochemical etching in which HF-free conditions were used to create MXenes such as $Ti_2CT_x$, $Cr_2CT_x$, and $V_2CT_x$ [126]. An electrode composed of three dimensions (3D) was utilized. The etching efficiency of MXenes was significantly increased by gently heating the MAX phase to accelerate the etching reaction in the presence of diluted HCl as the etchant. Given the widespread preparation of Ti-based MXenes, $Ti_2CT_x$ was chosen as a representative example for this investigation. $Ti_2CT_x$ was synthesized by a two-step electrochemical etching process [136].

Several morphologies of MXenes may be produced by adjusting the etching time, temperature, and electrodes [144]. Another two MXenes, $V_2C$ and $Cr_2C$, which were thought to be challenging to manufacture, may be effectively synthesized using this procedure [145]. According to earlier findings, $V_2C$ needed up to a 50 % HF concentration and HF corrosion for more than two days and the preparation of the $Cr_2C$ had been unsuccessful [146]. In addition to offering a general method for producing MXenes, thermally assisted electrochemical etching has also produced MXenes that are challenging to make. It provides a window for quickly, easily, and safely preparing MXenes.

### 7.4. Water-free etching

Lewis acid etching, also known as molten salt etching, and iodine aided etching are the two current non-aqueous etching techniques. Comparable to the reactions of $Ti_3A_lC2$ in molten $ZnC_{l2}$, the MAX phase in molten salt (Lewis acid) exhibited comparable characteristics to that of HF. By increasing the ratio of MAX: $ZnC_{l2}$, the $Ti_3ZnC_2$ MAX phase obtained by the substitution reaction was converted into $Ti_3C_2C_{l2}$ MXenes [147]. The Substitution-type reaction have been used to produce a class of Mn + 1 ZnXn phases after the reaction was optimized, leading to the surface-bound Cl group-containing matching (Mn + 1 XnCl2) MXenes [148].

Water-free etching, also known as dry etching, is a process used in semiconductor manufacturing and materials science to selectively remove layers of material from a substrate [149]. Unlike wet etching, which typically uses liquid chemicals (often aqueous solutions) to dissolve unwanted material, dry etching utilizes gas-phase etchants or plasma to achieve the same purpose without the need for water or other liquids [150].

The following techniques are involved in dry etching, including:

#### 7.4.1. Reactive ion etching (RIE)

In RIE, plasma is used to create chemically reactive species, such as ions and radicals, which react with the material being etched to form volatile byproducts. These byproducts are then removed from the surface, effectively etching away the material. RIE offers high anisotropy, meaning etching proceeds predominantly in the vertical direction, allowing for precise control over etch profiles.

#### 7.4.2. Inductively coupled plasma etching (ICP)

ICP etching is similar to RIE but typically operates at lower pressures and uses inductive coupling to generate plasma. This method can offer higher plasma densities and better control over ion energy, resulting in enhanced etch rates and etch selectivity.

#### 7.4.3. Deep reactive ion etching (DRIE)

DRIE is a specialized form of RIE used for deep, high-aspect-ratio structures, such as microelectromechanical systems (MEMS) and through-silicon vias (TSVs). It involves cyclic etching and passivation steps to achieve deep, precise etching profiles.

#### 7.4.4. Plasma etching

Plasma etching encompasses a variety of techniques where plasma is used to remove material. This can include techniques like electron cyclotron resonance (ECR) plasma etching and microwave plasma etching, among others.

Dry etching techniques offer several advantages over wet etching, including higher etch selectivity, better control over etch profiles, and compatibility with high-resolution patterning processes such as

photolithography. However, dry etching processes can be more complex and require specialized equipment, and certain materials may be more challenging to etch using dry techniques compared to wet methods [151].

With an increasing focus on green chemistry, researchers have created a number of economical and energy-efficient methods to create MXenes, or two-dimensional carbides and nitrides, from their parent MAX phases throughout the last ten years. Although safety and environmental concerns have prompted the search for alternatives, the most well-established technique, fluoride etching, removes the "A" layers and produces multilayered MXenes using either concentrated HF or in situ production of fluorinated etchants. While all the approaches listed in this section strikes a different balance between environmental effect, scalability, and efficiency, taken as a whole, they increase the toolkit for designing MXene's composition, morphology, and surface functioning to suit a range of application requirements.

## 8. Use of ML models to predict and optimize conditions for MXene synthesis for various applications

Advancements in MXene synthesis methods have greatly enhanced their electrical properties, physicochemical functionality, and versatility across various applications [152]. MXene synthesis is primarily categorized into two approaches: top-down and bottom-up methods [153]. The top-down approach involves extracting elements from parent three-dimensional (3D) layered MAX phases to produce the layered MXene structure [65]. This method is currently the most widely used for MXene synthesis. In contrast, the bottom-up approach begins by assembling MXene structures from small organic or inorganic molecules/atoms, offering precise control over size distribution, morphology, and surface terminations. For example, crystal growth techniques can construct well-defined 2D ordered MXene structures, allowing for tailored synthesis with superior uniformity [54].

Hydrofluoric acid (HF) etching—often combined with fluoride salts and hydrochloric acid (HCl)—is the most commonly employed technique among the top-down methods. Molten salt etching also provides a reliable alternative for MXene synthesis. These traditional approaches have been extensively reviewed in the literature [54]. Recent research has introduced advanced etching techniques, showcasing innovative fabrication pathways and intriguing physical properties of MXenes [154]. These cutting-edge methods pave the way for further refinement and broader application of MXenes in diverse fields. Fig. 7 describes the timeline evolution of the different synthesis methods and techniques used in recent years.

Lewis acidic etching has emerged as a promising technique for MXene preparation due to its mild production environment, making it well-suited for large-scale production and potential commercial applications [156]. Recently, innovative MAX phases such as $Ti_3ZnC_2$, $Ti_2ZnC$, $Ti_2ZnN$, and $V_2ZnC$ have been synthesized by replacing elements in the A atomic plane of traditional MAX phases using $ZnCl_2$ molten salts. Increasing the proportion of $ZnCl_2$ enables the production of Cl-functionalized MXenes (e.g., $Ti_3C_2Cl_2$ and $Ti_2CCl_2$) through direct redox coupling between the A element and the cation of the Lewis acid molten salt [46]. This method also facilitates the fabrication of MXenes from MAX phases with A = Ga and Si using $CuCl_2$ molten salts.

The moderate molten salt environment and fluorine-free conditions make this approach environmentally friendly and scalable, paving the way for commercial MXene applications [148]. Notably, this is the first method to produce exclusively Cl-terminated MXenes via non-fluorine chemistry, with Cl-terminated MXenes offering enhanced stability compared to their F-terminated counterparts [67]. Additionally, this approach allows the incorporation of various functional groups—such as -NH, -S, -Cl, -Se, -Br, and -Te—on MXene surfaces, enabling precise control over their surface chemistry, structure, and properties.

Despite significant progress, MXene research remains in its nascent stages. Although a wealth of reports on MXene fabrication has emerged over the past decade, certain theoretical aspects remain underexplored [65]. Many recently developed MXene materials are still in early developmental stages, suggesting that their properties may be underestimated due to suboptimal synthesis conditions. Emerging variants, such as $Mo_{1.33}C$ and $W_{1.33}C$, have demonstrated promising electrochemical performance and exceptional hydrogen evolution reaction activity, respectively. Additionally, less-studied MXenes like $Ta_3C_2$, $Ti_2N$, and $Cr_2Ti_2C_3$ have shown potential for applications in magnetic fields—a relatively underexplored area.

The introduction of novel synthesis methods and MXene variants has generated significant interest across multiple disciplines. Evaluating current preparation methods highlights several pathways for advancing MXene-based flexible devices, indicating vast potential for future innovation [157].

In energy storage, supercapacitors are pivotal electronic devices driving advancements in future technologies [15]. Their unique

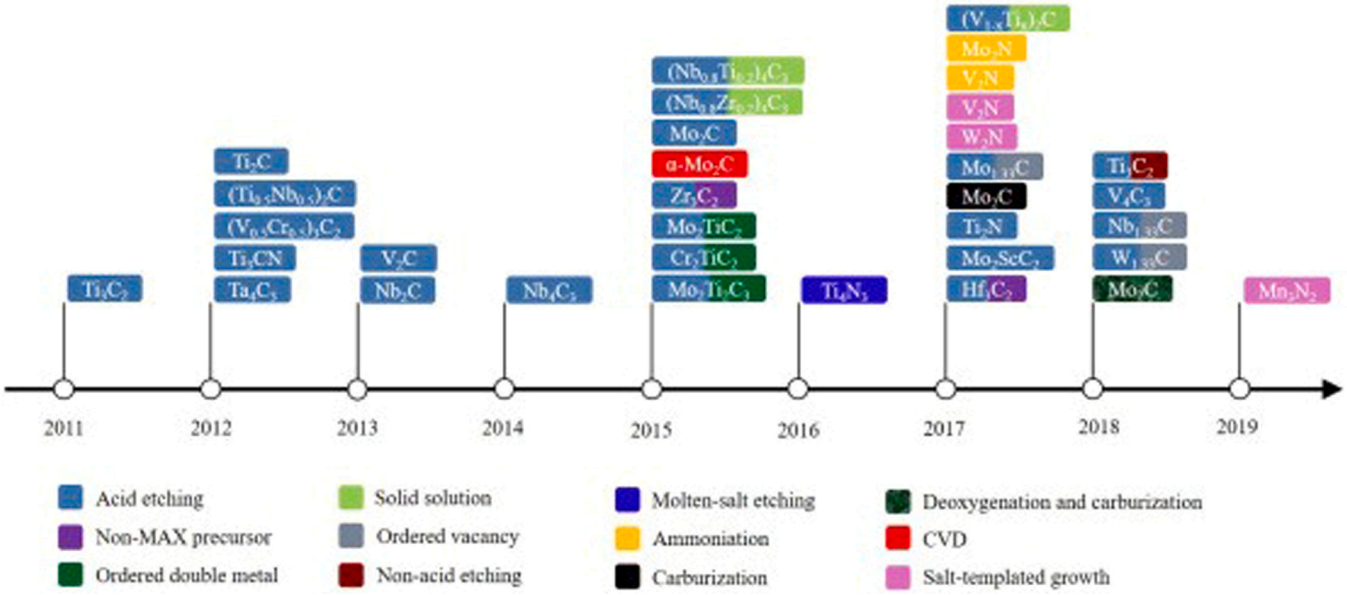



**Fig. 7.** Timeline of typical MXene synthesis methods in the Past Decade [155]. Culled with permission from Elsevier.

combination of high-power density, long cycle life, and rapid charge-discharge capabilities positions them as essential power sources for smart electronics, particularly in miniaturized devices [158]. Achieving the high energy density required for reliable performance in such applications depends on using materials with high capacitance, either through large surface areas or pseudo-active species.

Although graphene has been a primary focus in the study of 2D nanomaterials for supercapacitors, its limited energy density and capacitance have hindered its progress [159]. In contrast, 2D MXene nanomaterials provide a promising alternative, enabling efficient charge storage through cation adsorption and facilitating intercalation of water and electrolyte ions between their layered structures. MXenes exhibit unique properties, such as rapid expansion and contraction of their layers, enhancing charge storage. For instance, $Ti_3C_2T_x$ MXenes demonstrate a stable specific volumetric capacitance of nearly 1500 F $cm^{-3}$, outperforming all carbon-based supercapacitors [160]. Furthermore, many MXenes possess metallic conductivity, with values as high as 15,000 S $cm^{-1}$, ensuring rapid charge transfer and high current handling. These attributes have made MXene-based supercapacitor electrodes a focal point of research [161].

Flexible energy storage devices hold immense potential in modern electronics, including portable smartphones, wearable energy harvesting systems, and miniaturized storage devices [162]. Traditional sandwiched supercapacitors, limited by their bulkiness and low power density, face challenges in applications like micro power units for energy-intensive micro-electronic devices integrated on circuit boards. The advent of micro-supercapacitors (MSCs), featuring reduced size and simplified fabrication, enables their integration with other coplanar micro-electronic devices. This innovation has unlocked applications in wireless sensor networks, nanorobotics, micro-electromechanical systems (MEMSs), and flexible electronics [163].

Beyond their outstanding electrochemical properties, MXenes exhibit superior traits such as atomically thin layers, micro-scale lateral dimensions, and excellent hydrophilicity. These properties allow MXenes to form stable, viscous aqueous colloidal suspensions or inks without requiring surfactants or polymer additives, making them ideal for MSC electrodes [164]. To develop high-performance, durable MXene-based MSCs, it is crucial to engineer flexible electrodes that combine superior mechanical resilience with exceptional electrochemical performance [152].

## 9. Planar supercapacitors utilizing MXene

Conventional sandwich-like Micro-Supercapacitors (MSCs), with their considerable thickness, present challenges for achieving ultrathin device architectures, thereby limiting their integration into compact and wearable technologies. Recent advancements in micro-fabrication techniques have explored various physical and chemical methods to develop active materials for patterned interdigital MSCs [154]. The planar interdigital supercapacitor design incorporates electrode materials, electrolytes, and a current collector, with electrolytes filling the spaces between microelectrodes. Optimizing electrode spacing is crucial, as it reduces ion transmission distances and increases the effective electrode surface area, resulting in improved power and energy densities [50].

Conventional asymmetric supercapacitors (ASCs) have also contributed significantly to the advancement of energy storage. To enhance the performance of ASCs, a 3D architecture that increases interlayer spacing and enhances ion transport was created using a composite of MXene and a porous Ni-based MOF (see Fig. 8a), leading to better electrochemical performance than its constituent parts (as presented in Fig. 8b). The integrated electrode exhibited remarkable cycle

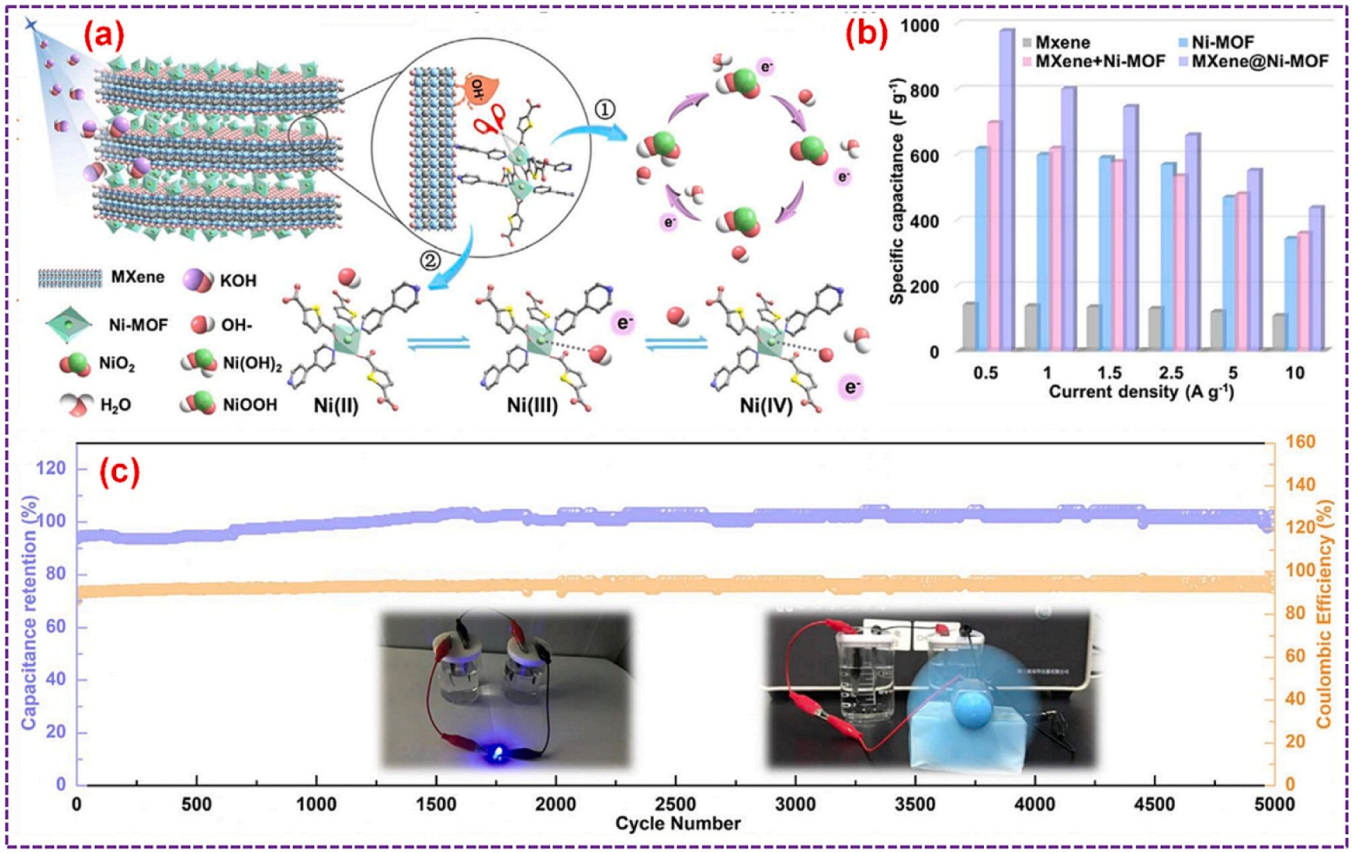



**Fig. 8.** (a) Pictorial representation of charge/discharge mechanism of MXene@Ni-MOF electrode. (b) Specific capacitance of Ni-MOF, MXene, MXene+Ni-MOF, and MXene@Ni-MOF electrodes. (c) Cycling stability of the MXene@Ni-MOF//AC device [165]. Culled with permission from Elsevier.

stability, maintaining the majority of its capacitance after 5000 cycles (Fig. 8c). Furthermore, different flexible MXene-based micro-supercapacitors have been developed for energy storage applications via manufacturing methods such screen printing, inkjet printing, and laser scribing.

## 10. Reinforcement learning and active learning in real-time process control

Reinforcement learning (RL) is a machine learning (ML) approach where an agent learns to interact with its environment through trial and error, guided solely by numerical rewards [166]. Machine learning is broadly categorized into three main paradigms: supervised learning, unsupervised learning, and reinforcement learning.

In supervised learning, the learning process relies on labeled data, where the relationship between input (X) and output (Y) is defined, enabling tasks such as classification and regression. The goal is to approximate the relationship $Y = f(X)$ using data-driven techniques like neural networks, achieving generalization and high accuracy for the given case study [89].

In contrast, unsupervised learning derives insights solely from the input features (X), without labeled outputs (Y). This paradigm focuses on discovering underlying structures in data, such as through clustering, and does not rely on a "teacher" to label effects [167].

Reinforcement learning (RL) distinguishes itself by learning autonomously without external supervision. It does not aim to learn the distribution of input data p(X) but rather seeks to identify the optimal strategy for accomplishing a task. This is achieved through iterative interactions with the environment, where the agent explores and refines its actions based on received rewards [168]. While RL's complexity requires analyzing multiple factors to define the problem effectively, it holds the potential to automate machine learning processes, expanding the scope of intelligent systems [9].

Active learning plays a crucial role in real-time process control, especially in the context of material prediction. In materials science, predicting material properties accurately is essential for designing advanced materials with specific functionalities. Traditional methods involve extensive experimental or computational efforts to gather data for training predictive models. Active learning, however, transforms this process by intelligently selecting the most informative data points for model training, thereby optimizing the learning process [169].

In real-time material prediction, active learning dynamically chooses data points based on the current state of the model and the uncertainty associated with its predictions. The goal is strategically picking data instances that contribute the most to reducing uncertainty or improving the model's accuracy [169]. This is particularly valuable when resources are limited, and acquiring additional data may be expensive or time-consuming.

The active learning loop typically begins with an initial set of labeled data points to train the material prediction model [170]. As predictions are made on new, unlabeled data points, the model evaluates its confidence or uncertainty in these predictions. Active learning algorithms then select instances where uncertainty is high, indicating areas where the model could benefit from additional information. These selected instances are labeled and incorporated into the training set, iteratively improving the model's accuracy over time. In real-time material prediction, active learning enables adaptive and targeted data acquisition [171]. Rather than relying on random or exhaustive sampling, the model actively guides the selection of experiments or simulations that will provide the most valuable information to refine its predictions. This iterative process continues, refining the model with each succeeding iteration and ensuring that the predictions become increasingly accurate and reliable [172].

The benefits of active learning in real-time material prediction extend beyond efficiency. By focusing on the most informative data, active learning accelerates the convergence of predictive models, allowing for quicker adaptation to evolving conditions or changing requirements [173]. This adaptive learning approach is particularly advantageous in dynamic research environments, where continuous improvement and optimization of material prediction models are essential for staying at the forefront of materials discovery and development.

Reinforcement learning (RL) and active learning are innovative approaches that hold significant potential in real-time process control, particularly in synthesizing MXenes, a class of two-dimensional materials with diverse applications [174]. MXenes are typically produced through complex and multistep processes and optimizing their synthesis parameters in real-time is challenging. Reinforcement learning, a branch of machine learning, offers a dynamic solution by allowing an agent to learn optimal actions in an environment to achieve a specified goal. In the context of MXene synthesis, RL algorithms can adaptively adjust various synthesis parameters, such as temperature, reaction time, and precursor concentrations, to maximize the yield, quality, or desired properties of the synthesized MXenes [70]. On the other hand, active learning focuses on selecting informative data points to train a model effectively. In MXene synthesis, active learning can be employed to guide the experimental design process [57]. By strategically choosing specific experiments or simulations based on the current knowledge, active learning ensures that the model is continually improved with minimal resource utilization. This is particularly advantageous in MXene synthesis, where experimentation can be time-consuming and resource-intensive [163]

Integrating reinforcement learning and active learning in real-time process control for MXene synthesis involves creating a closed-loop system [175]. The RL agent, responsible for adjusting synthesis parameters, interacts with the MXene synthesis process in real time [176]. The agent receives feedback on the outcomes of each synthesis, such as the quality and yield of the MXenes, and learns from this feedback to make more informed decisions in subsequent experiments [177]. This combined approach addresses the challenges associated with MXene synthesis, where the optimal conditions are often complex and multifaceted. RL and active learning empower the system to adapt and learn from the evolving synthesis conditions, ultimately leading to improved efficiency, reduced experimentation time, and enhanced control over MXene properties [178]. The real-time adaptation and learning capabilities of these approaches make them valuable tools in the quest for efficient and optimized MXene synthesis processes.

## 11. Improving MXene yield and purity through ML-assisted synthesis

Applying machine learning to screen extensive material databases to identify suitable electrocatalyst properties presents notable benefits, including improved yield, purity, and reduced experimental cycles and costs. It helps address the intricate challenge of material selection. Using 2D materials with increased active sites holds significant promise for large-scale hydrogen production, aiming to replace Pt catalysts [58, 179]. Swiftly identifying high-performance 2D Hydrogen Evolution Reaction (HER) catalysts faces substantial obstacles due to prolonged experimental cycles and elevated costs associated with high-throughput calculations for adsorption energies [180]. There is a growing interest in MXene-based materials, notably for their potential applications in the HER [181]. For example, the 2D metal carbide semiconductor $Ti_2CO_2$ MXenes, featuring a cost-effective basal plane, has been employed as electrocatalysts for the HER. As depicted in Fig. 6(a-c), the HER performance of these MXenes can be finely tuned by immobilizing single transition metal (STM) atoms onto Ti vacancies. Materials in 2D with more active sites exhibit significant potential for large-scale hydrogen production, poised to replace Pt catalysts. However, the rapid discovery of high-performance 2D catalysts for the hydrogen evolution reaction (HER) is hindered by prolonged experiment cycles and high costs associated with high-throughput calculations for adsorption energies

[182,183]. MXene-based materials, particularly, are gaining considerable attention due to their potential applications in HER. For example, the 2D metal carbide semiconductor $Ti_2CO_2$ MXenes, featuring a cost-effective basal plane, has been employed as electrocatalysts for the HER. The HER performance of these MXenes can be modulated by immobilizing single transition metal (STM) atoms onto Ti vacancies [184]. Peng et al. [184] explained that on several occasions, ML models were employed to discover 27 distinct MXenes $Ti_2CO_2$-STMs and 81 HER catalytic active sites based on a facile descriptor.

In order to effectively screen and create high-performing HER electrocatalysts MXenes, Yang et al. [185] synthesized a V-based non-metal doped and combined machine learning (ML) with high-throughput density functional theory (DFT) calculations. The top and side views of the non-metal doped MXenes are shown on Fig. 9. Analysis reveals several non-equivalent active spots on the surface, designated $S_0$, $S_1$, and $S_2$ (Fig. 9). Following NM atom doping, S0, S1, and S2 stand for three non-equivalent H adsorption sites. There is a chance for increased catalytic activity due to the increase in active sites.

They chose 15 descriptors that represent important material characteristics, including charge description, bond length, and electronic structure, which may be connected to the catalytic activity of NM-V2CO2 and NM-V2CS2. The correlation of the descriptors was determined using the calculated Pearson correlation heatmaps of the matrix, which are displayed in Fig. 10(a). Only one of the nine features—which are clusters of strongly correlated variables—is kept for model training out of the fifteen features. The model scores obtained by various algorithms when choosing the two top feature; the distance between the adsorption site and V and the Pz band center of the adsorption site were shown in Fig. 10(b). These descriptors performed steadily and consistently over a range of models. The GBR model produced higher R2 (0.990 for training set and 0.980 for testing set) and lower RMSE (0.081 eV for training set and 0.094 eV for testing set) scores in comparison to the ABR and GBR algorithms. The GBR model features are examined in Fig. 10(c, d), which also shows the error scores for varying feature counts and the GBR ranking results for the top five features. The two characteristics clearly play a major role in ΔGH*. The model error minimizes overfitting by plateauing beyond the top two features as the number of features increases. Fig. 10(e) compares the ΔGH* predicted by the GBR algorithm and the DFT calculation. The training set's (red) and the testing set's (green) computed/predicted values are shown to be substantially consistent. This suggests that the catalytic activity of NM-V2CO2 and NM-V2CS2 may be reliably predicted by the GBR model. The universal descriptor $\psi = dV\text{-}ado^2 \times (dV\text{-}ado - \varepsilon pz\ ado)$ is then extended in Fig. 10(f) and (g) to predict ΔGH* in $V_2CO_2/S_2$ and $V_2CSe_2$ systems, respectively, with $R^2 > 0.94$. Lastly, Fig. 10 (i) confirms the transferability of ψ by correctly predicting ΔGH* for NM-$Ti_2CO_2$. Fig. 10 (h) uses ψ to screen NM-doped $V_2CTe_2$, emphasizing dopants that bring ΔGH* within the ideal ±0.2 eV window. For better yield and purity, Fig. 10 demonstrates how ML-driven feature selection and symbolic regression may quickly identify the critical parameters required to direct experimental synthesis. This allows for targeted optimization of MXene manufacturing settings.

## 12. Conclusion and future prospects in MXene materials

The knowledge, design, and use of MXene can be greatly advanced by applying machine learning (ML) to its compounds. MXenes are a type of 2D transition metal carbides, nitrides, and carbonitrides that have attracted a lot of attention because of their remarkable qualities, which include changeable surface chemistry, high conductivity, and mechanical strength. Predicting and designing properties through large databases of MXene properties may be used to train machine learning algorithms, allowing them to anticipate new materials with desired qualities. Machine learning algorithms help to comprehend the complex structure-property relationships observed in MXene materials by analyzing experimental and computational data. The time and resources needed for materials development can be decreased by using machine learning (ML) models to direct experimental efforts toward promising candidates with improved performance metrics by utilizing computational simulations. Machine learning models can facilitate the identification and refinement of MXene-based materials for a variety of applications, including sensing, energy storage, and catalysis, by establishing a correlation between the composition, structure, and processing conditions of MXene and properties like thermal stability, electrochemical performance, and electrical conductivity.

This review identifies different unique machine learning models that have been applied in predicting the MXenes' properties and their commercial applications. This work also addressed the problems associated with MXene synthesis and appraised the possibility of using machine learning in the synthesis, modifications, and application of MXenes in battery, supercapacitor, absorption of materials, water purification, and catalysis.

The use of ML models to reduce production cost and determine the ideal conditions for MXene synthesis in an industrial scale remains an open research area. Studies based on the scalability, economics of MXenes fabrication methods, and development of ML-powered materials informatics platforms is identified as the future direction of research in MXenes materials. The use of ML algorithm in expanding the applicability of MXenes especially in the electronic industry is another area expected to lead MXene research in the future.

MXenes' exceptional qualities, including their electrical conductivity, mechanical strength, and thermal stability, make them extremely

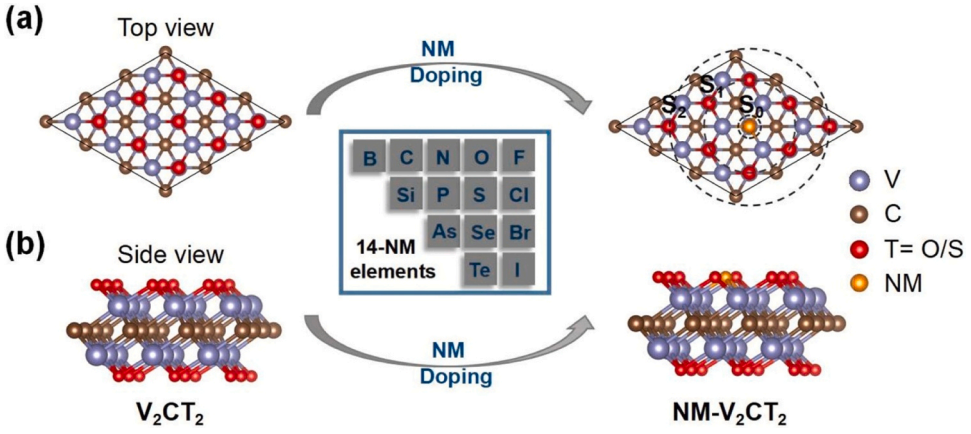



**Fig. 9.** Top and side views of 3 × 3 × 1 supercell of 2D $V_2CT_2$ and NM-$V_2CT_2$ (T = O, S) crystal structures. (a) Top view for MXenes. (b) Side view for MXenes[185]. Culled with permission from Elsevier.

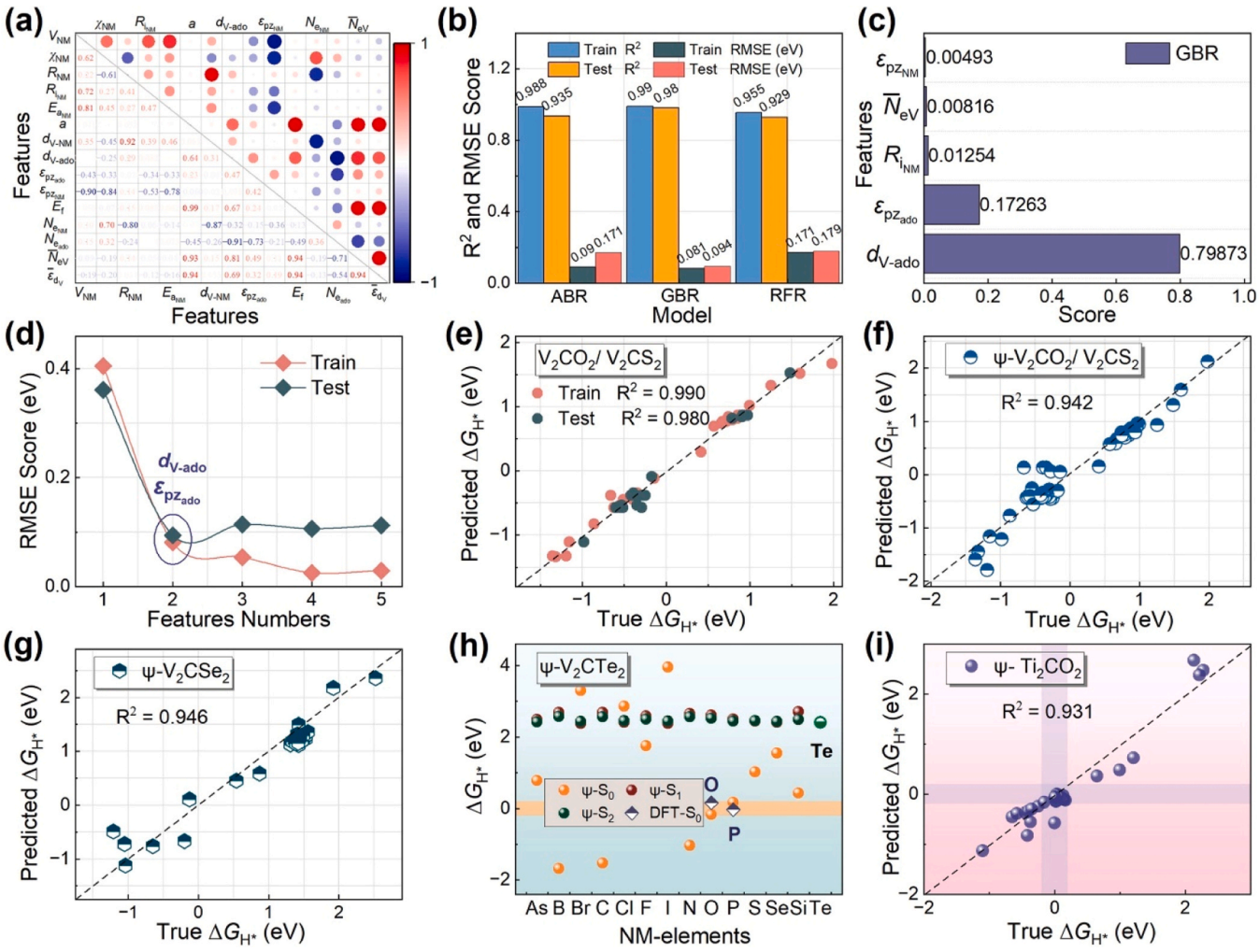



**Fig. 10.** (a) Correlation map of the 15 features. (b) The scores of 2 top ranked descriptors of training and testing sets for ABR, GBR and RFR, respectively. (c) The importance distribution of the top five ranked features for GBR. (d) The error scores for different number features for GBR; (e) Comparison between ML predicted and DFT-calculated of $\Delta G_{H^*}$ for GBR. (f) New descriptor ψ performance for NM-$V_2CO_2$ and NM-$V_2CS_2$. (g) New descriptor ψ performance for NM-$V_2CSe_2$. (h) DFT Validation and new materials exploration in NM-$V_2CTe_2$. (i) New descriptor ψ performance for NM-$Ti_2CO_2$[185]. Culled with permission from Elsevier.

appealing for a variety of uses, from electronics and energy storage to catalysis and the biomedical industry. However, issues with scalability, surface functionalization, and basic comprehension need to be resolved in order to fully realize the potential of MXenes. Enhancing synthesis methods, streamlining procedures, speeding up materials discovery, and creating MXene-based materials with superior properties for a variety of applications are all made possible by the integration of AI in every stage of design and properties evaluation of these MXene materials.

The electrical, optical, thermal, and mechanical properties of MXenes that are suited for certain applications can be predicted and optimized by AI algorithms based upon their processing parameters, compositions and even down to their atomic structures. Furthermore, by evaluating current data and proposing creative strategies or alterations to conventional synthetic methods, AI can aid in the creation of novel synthesis procedures for MXenes, increasing synthesis efficiency, scalability, and reproducibility. Crucially, ML models are excellent at deciphering and evaluating intricate MXenes characterisation data. ML models can be used to gain a deeper understanding of MXene structures and properties by using different data-driven models approaches to extract valuable insights from spectroscopic, microscopic, and diffraction data. Applications of ML models also make it possible to virtually screen and optimize MXenes using computational modeling, giving researchers the ability to investigate a wide range of MXene compositions and structures. This speeds up the process of finding materials with the right qualities for certain uses. In order to help researchers make well-informed decisions, the use of ML models and AL algorithms can synthesize and analyze a vast amount of MXene-related literature, patents, and experimental data to create a comprehensive knowledge base. Within this knowledge base, AI algorithms can suggest possible synthesis strategies, applications, and research directions. In order to ensure the consistency and superior quality of MXene materials, machine learning models can be used to monitor and evaluate a variety of quality control parameters throughout the synthesis of MXene. This allows for the real-time detection of process irregularities or flaws.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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