

Review article

Synthesis and application of double metal MXenes: A review



Asieh Akhoondi ^(D) ^{a,*}, Mitra Ebrahimi Nejad ^{b, c,*}, Mohammad Yusuf ^(D) ^d, Tejraj M. Aminabhavi ^(D) ^e, Khalid Mujasam Batoo ^(D) ^f, Sami Rtimi ^(D) ^{g, h}

^a Department of Chemical Engineering, Arak Branch, Islamic Azad University, Arak, Iran

^b Chemical Engineering Faculty, Tarbiat Modares University, P.O. Box 14115-111, Tehran, Iran

^c Cracking and Catalysis Research Center, Tarbiat Modares University, P.O. Box 14115-111, Tehran, Iran

^d Clean Energy Technologies Research Institute (CETRI), Faculty of Engineering and Applied Science, University of Regina, 3737 Wascana Parkway, Regina, SK S4S 0.42, Canada

^e School of Advanced Sciences, KLE Technological University, Hubballi 580031, India

^f King Abdullah Institute For Nanotechnology, King Saud University, Riyadh-11451, Saudi Arabia

^g Ecole Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

^h Global Institute for Water, Environment and Health (GIWEH), 1210 Geneva, Switzerland

ABSTRACT

MXenes are known as a new type of two-dimensional layered materials that are composed of carbide, nitride, or carbonitride of transition metals. In the recent discovery of a new class of MXenes, two transition metals occupy the metal site, called double transition metal MXenes (DTM). These multilayer composites are of interest due to their attractive features such as high ion transport, extensive surface area, and biocompatibility. Some computational methods are used to predict the properties and performance of bimetallic carbonitrides. The most important feature of this category of materials is the stability and amount of formation energy, which directly affects the choice of material in various applications. Density functional theory (DFT) calculations are very beneficial to estimate the thermodynamic stability of DTM MXenes. Of course, proper surface modification with stable terminals is needed to overcome the limitations of DTM MXenes. In this review, the electrochemical, metallic, and magnetic properties of DTM MXene have been presented first. In the following, preparation methods are summarized according to the latest published findings. Then, various applications including hydrogen evolution reactions, anode materials in lithium and sodium batteries, nanomagnetic materials, and special applications have been investigated. Finally, more challenges, prospects, and suggestions for the development of two-dimensional DTM MXenes have been presented. © 2023 The Authors. Published by Synsint Research Group.

1. Introduction

The two-dimensional structures or single-layer materials have significant differences in specific surface area, basic properties, and optical output (wavelength, intensity) compared to their counterpart solids [1]. 2D crystals such as graphene have received great attention in material science and engineering at the nanoscale, especially in semiconductors [2]. In two-dimensional materials, by reducing the thickness of the material even to one atom, major changes can occur in their properties [3]. Therefore, extensive studies have been conducted on the atomic structures, mechanical properties, behaviors, and defects of two-dimensional materials, which are the basis for their practical

KEYWORDS



^{*} Corresponding author. E-mail address: asieh.akhoondi@gmail.com (A. Akhoondi), mitra.ebrahimi@modares.ac.ir (M. Ebrahimi Nejad)

Received 27 May 2023; Received in revised form 27 June 2023; Accepted 28 June 2023.

Peer review under responsibility of Synsint Research Group. This is an open access article under the CC BY license (https://creativecommons.org/licenses/by/4.0/). https://doi.org/10.53063/synsint.2023.32150

applications. It is predicted that thousands of crystals can be established from various solids by exfoliation, which is classified as twodimensional materials [4].

In 2011, two-dimensional inorganic compounds called MXenes with the general formula $M_{n+1}X_nT_x$ were found from the family of transition metal carbides and nitrides atomically thin layers [5]. In the $M_{n+1}X_nT_x$ (n=1–3) systems, M is a transition metal and X is either C and/or N, terminated with T: –O, –F, –OH, and –Cl or bare. MXenes are synthesized through selectively acidic etching of the MAX phases ($M_{n+1}AX_n$, n=1–4), where A is an element of groups IIIA or IVA of the periodic table. A is mostly Al or Si in the layered hexagonal structure of MAX phases which is eliminated by HF acid [6]. At present, a large number of MXenes have been reported such as Ti₂CT_x, Ti₃C₂T_x, Nb₂CT_x, Nb₄C₃T_x, V₂CT_x, Ta₄C₃T_x, etc. [7]. While mainly titanium, niobium, and vanadium form the structure of MXenes, other metal elements such as Sc, Zr, Hf, and Mo are also predicted to form MXenes [8, 9].

Since MXenes have a high surface area per unit weight and electrical conductivity and hydrophilicity are their fundamental properties, they have found potential applications, especially in energy storage [10]. The ability to adjust the surface terminals of this type of twodimensional materials has created a promising future in the preparation of thermoelectric devices [11], composites [12], photocatalysts [13], sensors, electrodes, batteries [14], nano-magnets, supercapacitors [15], and membranes. The semiconductor nature and unique physicochemical properties of these compounds have led to their use in photocatalysis in order to accelerate redox reactions such as hydrogen evolution reactions and other photocatalyst-based usages [16]. Moreover, as two-dimensional emerging materials, MXenes have potential applications in biomaterials nanomedicine [17], and photothermal conversion [18].

In the group of MXenes, other solutions have been invented; where two transition metals occupy the M positions which differ from their single transition metal counterparts [19]. The two intermediate metals are distinguished by M' and M" and these semiconductors are divided into

in-plane and out-of-plane groups (ordered DTM MXenes), and solidsolution DTM MXenes based on their structure. The behavior of these three groups of DTM MXenes is different from single metal MXenes, which can have various uses in the future. The purpose of this review is to investigate the characteristics, design, and synthesis methods of double-transition metal MXenes (DTM) and their hybrids in composite configuration with growing applications from electrocatalyst to energy storage.

2. Basic properties

MXenes have a high stability because they are synthesized under strongly acidic (HF) conditions [20]. It should be noted that the stability in bimetallic MXenes depends on the type and content of each of the constituent metals. For instance, in Fig. 1, the stability of $Mo_xV_{4,x}C_3$ is shown for different values of x [21]. According to this figure, V_4C_3 is stable throughout the molybdenum-containing region. Moreover, MXenes offer a unique combination of metallic conductivity and hydrophilicity that have already shown promise as electrodes for supercapacitors and Li-S batteries. The developed composites based on carbonitride MXenes have high resistance under high-temperature oxidation [22]. In this regard, TiCrC with a Ni-Cr additive has been investigated. It has been recommended that cladding technology with a Ni-P alloy be used to decrease the intensity of the composite oxidation. In addition, MXenes have a large surface area and high electron mobility, which promises a wide range of applications in the future.

The results of DFT calculations and experimental methods have shown that doubly ordered carbonitrides are thermodynamically more stable than solid solution counterparts [8]. The characteristics and properties of DTM MXenes are distinguished among existing 2D materials by carefully engineering the composition, the number of metal sheets, interlayer space, and terminated group functionalities [23]. Furthermore, the electronic thermal conductivities of DTM carbonitrides revealed by Boltzmann's transport theory differ with single metal MXenes. In one case, the Ti layers have been covered with



Fig. 1. Phase diagram for the thermodynamic stability of the different Mo_xV_{4-x}C₃ MXenes.



Fig. 2. Electrical and thermal conductivities variations of Y₂ScC₂O₂, Sc₂YC₂O₂, Y₂TiC₂O₂, and Ti₂YC₂O₂.

Y atoms in Ti₃C₂O₂ to modify the electronic structure and transport characteristics [24]. In addition, TiY₂C₂O₂ MXene has higher electrical conductivity compared to Ti2YC2O2 because of its squared band velocity. This phenomenon also applies to Sc₂YC₂O₂ and ScY₂C₂O₂, whose functional group is -O (Fig. 2). On the other hand, Chang et al. [25] calculated the semiconductor properties of ScYCT₂ (T: F and OH) and bandgap and believe that ScYCF2 and ScYCOH2 are stable and has better thermoelectric properties. In another study, Caffrey [26] has shown the effect of different types of terminating groups on the stability of DTM MXenes. In his research, it was found that Mo2Ti2CTx is stable in a wide range of pH in aqueous solution. In contrast, Cr₂Ti₂CT_x and Cr₂V₂CT_x are only stable at pH<7 when T is restricted to the -F functional group. But in the case of Mo₂Sc₂CT_x, if scandium ions interact with F ions in the solution and form ScF₃, this MXene cannot be stable under acidic pH. In addition, Mo₂ScC₂ and its functionalized congeners meet the criteria of mechanical stability. If oxygen is the surface terminal, it can be a suitable option for ultrasensitive sensors [27].

According to a comprehensive evaluation of surface modification,

Dihingia et al. [28] have found that –O functionalized carbonitrides are the most durable systems (Fig. 3). The second stable group is the fluorine surface functional class, and MXenes with –OH terminal are the least stable types except for the W-based/MoCr₂ carbide and nitride compounds. It has been experimentally proven that 2D materials have almost all the properties observed in bulk materials except magnetic behavior [29]. As two-dimensional composites, MXenes have great potential to achieve intrinsic magnetism due to their chemical and structural diversity [30].

3. Synthesis and design

Since DTM carbonitrides can be pristine or with multiple surface end groups, they have many varieties. The type of pair of transition metals greatly affects the energy of formation [31]. Geng et al. acknowledged that MXene monolayers with oxygen functional groups are easily constructed due to low formation energy (E_r), while M₂M'C₂ with boron end groups have the highest formation energy [32]. Most M₂M'C₂ functionalized with N, S, and P have positive or negative



Fig. 3. The adsorption energies of terminated systems with -OH, -F, and -O groups onto the surfaces of Cr-Mo, Cr-W, and W-Mo MXenes.



Fig. 4. Top and side view of 2D M₂M'C₂ and the formation energies of Mo₂TiC₂T_x, Mo₂VC₂T_x, Cr₂TiC₂T_x, and Cr₂VC₂T_x monolayers.

formation energy except Mo₂VC₂N₂, Cr₂VC₂S₂, and Cr₂MC₂N₂ with top Ti and V configuration (Fig. 4). Alternatively, E-etching (electrochemical etching) offers a favorable, practical, fast, and environmentally gentle technique for aluminum removal [33]. In the following, various synthesis routes of DTM MXenes are summarized. In one case, the different elemental molar ratios of Nb:Mo have been mixed with a constant molar ratio of Al:C and sintered at high temperatures for several hours under argon flow to achieve MAX phases [34]. After the successful exfoliation of aluminum layers in MAX phases to produce $Mo_{2+0}Nb_{2-0}C_3T_x$, two strategies can be used to convert MXene layers into flake-shaped monolayers: 1) utilization of HF/HCl with delamination agent (LiCl) and 2) solution of HF/tetramethylammonium hydroxide (TMAOH). Flake sizes of different $Mo_{2+0}Nb_{2-0}C_3T_x$ synthesized HF/TMAOH are shown in Fig. 5 with the comparison of the current density of Mo_2CT_x and $Mo_{1.33}CT_x$ produced from references [35] and [36]. The $Mo_{2.5}Nb_{1.5}C_3T_x$ has the highest electrical conductivity even more than bare $Mo_2Ti_2C_3T_x$, indicating some changes in the electronic structure.

MAX phases contain strong layer bonds that require a strong etch. The synthesis of carbonitrides can be achieved through a wet chemical method for etching selective layers from their precursor MAX phase at RT or above. In the research conducted on the charge transfer resistance of $Mo_2TiC_2T_x$ and $Mo_2Ti_2C_3T_x$, the wet chemical method has been used for synthesis in a Teflon bottle containing HF immersed in an oil bath [37]. The etched powder has been stirred, washed, and centrifuged to obtain exfoliated MXene. Electron impedance spectroscopy (EIS) of $Mo_2Ti_2C_3T_x$ has shown higher charge transfer resistance than $Mo_2TiC_2T_x$ (Fig. 6). Hence it is predicted that $Mo_2TiC_2T_x$ has a rapid kinetic and better catalytic performance for HER and OER.



Fig. 5. a) Flake sizes of $Mo_{2+\theta}Nb_{2-\theta}C_3T_x$ prepared through HF-TMAOH etching and b) potential vs. current density plots of $Mo_2Ti_2C_3T_x$ and $Mo_{2.28}Nb_{1.67}C_3T_x$ compared to Mo_2CT_x and $Mo_{1.33}CT_x$.

The hydrothermal method is one of the most powerful and widely used for the production of nanostructures, which has received a lot of attention today due to its simplicity and cost-effectiveness [38]. As is known from the name of this method, the synthesis based on the formation and growth of crystals, takes place in water at a moderate or high temperature above RT [39]. Therefore, Ma et al. [40] adopted this method in order to deter the destruction of the original layered construction of MXene after etching with hydrofluoric acid to prepare TiNbC MXene. Hydrothermal pretreatment on TiNbCT_x also prevents abnormal grain growth by direct calcination in the air. Next, the TiNbC suspension is freeze-dried to obtain black powder. The variables in the hydrothermal process are the type of water, temperature, time, surfactant, and pH, which have key roles in product quality [41]. The ratio of Nb to Ti in Ti-Nb carbides significantly influences the fabricated composition, but it does not have a direct relationship with the stoichiometry of MXene [42]. The TiNbC colloidal precipitate with Nb and TiO₂ is placed in an insulated container to synthesize Nb-doped TiO₂/TiNbCO as a new type of composite at high temperatures for several hours. In the following, the output solution from the autoclave is heated in an oven to get the final powder [43]. The degree of oxidation of TiNbC can be tuned by temperature controlling, and the oxide nanolayers turn dense with the increase in temperature. The strength junctions of TiNbCO and Nb-doped-TiO₂ nanosheets are ensured through the in-situ partial oxidation [44]. Moreover, the components' synergy and electrochemical activity are improved with double metal MXene and metal oxide [45]. However, it has been found that the electrical conductivity and hardness of the TiNbC composite that is combined with SiC significantly increases [46]. To investigate



Fig. 6. Electron impedance spectroscopy together with fitted equivalent circuits of Mo₂Ti₂C₃ and Mo₂TiC₂.

the properties of TiNbC-SiC composite, Fides et al. used the hot pressed method for synthesis in two steps without adding sintering additives. The results of electrical discharge machining (EDM) of the samples indicate the readily machinable composite but severe oxidation of the cuttings, which indicates that more surface treatment is needed. In another research, Andrade and co-workers [47] synthesized solid solution Nb_yV_{2-y}C by selective etching of niobium and vanadium with a controlled ratio, next by oxidation and dissolution in H_2O_2 and recrystallization by hydrothermal process. They demonstrated the construction of a solid solution boosted the etching kinetic of MAX phases and facilitated the carbide formation compared to pristine V and Nb MXenes.

In another study, Mo2TiAlC2 powder was used in an aqueous concentrated hydrofluoric acid to prepare Mo₂TiC₂T_x MXene [48]. After mixing and washing with distilled water, the obtained solution was centrifuged to reach the desired acidity (pH=6-7). Next, the water in the suspension is completely removed by the freeze-dried method. For the exfoliation of Mo₂TiC₂T_x, (C₄H₉)₄NOH as an organic solvent has been used. After stirring for one day, the solution was centrifuged and washed with water to eliminate the solvent. The synthesis method of Mo₂TiC₂T_x-molybdenum vacancy (V_{Mo}) is an electrochemical exfoliation technique in which the deposition of $Mo_2TiC_2T_x$ on an electrode serves as the working electrode. Meanwhile, by creating molybdenum vacancies, platinum atoms can be anchored in their place. In order to prepare Mo₂TiC₂T_x-single Pt atoms (Pt_{SA}), in-situ electrochemical exfoliation and atom trapping strategy have been employed in a three-electrode system. The XANES measurement of the electronic state of the Pt species in Fig. 7a exhibits higher intensities of Mo₂TiC₂T_x-Pt_{sA} compared to Pt foil and PtO2. Fig. 7b shows the Fourier transforms of the Pt edge, which indicates Mo₂TiC₂T_x-Pt_{SA} has no Pt particles or clusters.

4. Applications

4.1. Hydrogen evolution

Sustainable producible clean hydrogen is a promising alternative energy carrier to replace carbon-based fuels [49]. Hydrogen production by water splitting with an electrocatalytic approach can become more sustainable after discovering new materials, such as 2D nanomaterials [50]. Developing environmentally friendly, low-cost, stable, and highly active catalysts for the non-precious hydrogen evolution reaction (HER) is one of the critical factors for the hydrogen energy economy [51]. Double-transition-metal MXenes (DTM MXenes) have been widely pursued in the advancement of renewable energy storage technology in recent years [52]. It seems that the T_x terminal groups play an effective role in expanding the hydrogen production reaction, which is attributed to the interaction of MXene with the reactants and the creation of more active sites [10]. However, there is still insufficient information on the electrochemical characteristics and thermal stability of bimetallic MXenes. Since pure M'2M"C2 carbonitrides are surrounded by metal atoms and free electrons, the end terminals easily become electronegative during synthesis, which plays a significant role in charge transfer for hydrogen evolution reaction [10].

Based on the density functional theory (DFT) calculations of Li et al., the performance of mono-metal MXenes is improved by forming a sandwich configuration of double-metal MXene [52]. The results of their research showed that in terms of hydrogen production, carbonitrides made of molybdenum (Mo2M"C2O2) are more efficient than chromium-based MXene (M": Ti, V, Nb, and Ta). As a result of improving the geometric structure, the activity of MXenes promotes the direction of the hydrogen evolution reaction. The ΔG energy of H* adsorption and hydrogen coverage exhibits an intimate relationship to the H₂ production of carbonitrides. Through DFT calculations, Zeng and colleagues have found 11 candidates superior to platinum among 64 ordered DTM oxygen-functionalized MXenes for hydrogen production [53]. Furthermore, Mo₂TiCNO₂, Ti₂VCNO₂, and Ti₂NbCNO₂ have been screened in terms of stability compared to other compounds of this group of MXenes. Among these three compounds, Ti₂NbCNO₂ is more capable of catalytic conversion because it has abundant catalytic sites in carbon and its ΔG is lower in hydrogen absorption. In another research, it has been found the ΔG of H₂ absorption of Mo2TiC2P2 and CrM'C2S2 (M': Ti and V) with spontaneous conductivity are close to zero, which is a requirement for high catalytic activity in hydrogen production [32]. The difference between the energy level in the vacuum and the Fermi level is known as the work function [54]. In other words, the work function provides



Fig. 7. a) Normalized XANES spectra of Mo₂TiC₂T_x-Pt_{SA} and b) the Fourier transform of EXAFS spectra.



Fig. 8. a) Work function of $M_2M'C_2T_2$ monolayers and b) Volcano curve of exchange current vs. ΔG_{H} .

an energy barrier against the free space preventing electrons in the Fermi level. As seen in the Fig. 8, terminal atoms can affect the performance of carbonitrides. Functional group -O shows the highest work function in M₂M'C₂ monolayers, which strongly connect with internal electrons.

By examining the surface functional group, Sun and colleagues [55] discovered that DTM MXenes can be made semiconducting. In this regard, TiMn₂N₂–F has a wide range of properties, which has encouraged practical studies in wide applications. It has been found that TiMn₂N₂F₂ is half-metallic with a large bandgap of ~1.1 eV. In another work, O-functionalized DTM carbides have been investigated to estimate elastic, and electronic properties by DFT calculations [56]. It has been found that the elastic features of Mo-based C_2O_2 are superior compared to Cr-based counterparts. In addition, the O-terminated carbides have shown enhanced shear moduli, Young's moduli, and elastic constants compared to the unfunctionalized family. According to a recent theoretical study by Jin et al. [57], it has been

determined that the introduction of oxygen vacancies can increase the stability of DTM MXenes modified by a mono metal component such as Au, Ag, Pt, Zn, Cu, Ni, and Co. The stability of surface atoms added to MXenes increases with the introduction of oxygen vacancies, and also ΔG of hydrogen adsorption with metal atoms is adjusted. The reaction mechanism of H₂ desorption changes with the presence of metal atoms and removes the obstacles to the activation of hydrogen production, which leads to the improvement of the catalytic activity. In other research, Zhang et al. [48] have utilized single Pt atoms on Mo₂TiC₂T_x with abundant Mo vacancies to promote the efficiency of catalytic hydrogen evolution. Single atoms trap with the molybdenum vacancy on MXene nanosheets (NSs) and the kinetics of H2 production is similar to hydrogen evolution by commercial Pt-carbon catalyst. Fig. 9 shows the polarization curve of $Mo_2TiC_2T_x$ with platinum (counter electrode) in order to produce hydrogen in several cycles. Among all samples tested, the Mo₂TiC₂T_x/Single Pt atom shows the highest performance, competing with the Pt-carbon catalyst. In



Fig. 9. a) HER polarization curves of $Mo_2TiC_2T_x$ with platinum and b) calculated the free energy profile of HER at the equilibrium potential.

addition, due to the strong covalent interaction between charged platinum atoms and the DTM MXene, this compound exhibits high stability and prevents material aggregation during H_2 evolution. Moreover, Pd/Mo₂TiC₂T_x hybridized with MoS₂ is sufficiently active for electrocatalytic hydrogen evolution in acidic and alkaline electrolytes [58].

Although MXenes are superior to noble metals in water electrolysis for green H₂ production, coordinating both hydrogen and oxygen evolution reactions (OER) is still a challenge. Therefore, Zahra et al. [37] have investigated the dual performance of two types of DTM MXene as an electrocatalyst in alkaline media for overall water splitting. In this regard, they focused on the synthesis of Mo₂TiC₂T_x and Mo₂Ti₂C₃T_x via the wet chemical method. Mo2TiC2Tx has shown better oxygen evolution activity with lower overpotential than Mo₂Ti₂C₃T_x. Another molybdenum-based DTM MXene is $Mo_{2+\theta}Nb_{2-\theta}C_3T_x$ (0<0<0.3) with tunable performance for H₂ evolution reaction [34]. It is predicted that Mo-Nb carbonitrides are stable when niobium ions occupy the inner sites according to the Mo-C-Nb-C-Nb-C-Mo arrangements. Among the $Mo_{2+\theta}Nb_{2-\theta}C_3T_x$ derivatives for catalytic hydrogen production, Mo_{2.28}Nb_{1.6}7C₃T_x has the lowest excess potential. In another work, ZIF-67 derived C-N co-doped spongy Co₂P heterostructure has been anchored on Ti₂VC₂T_x for electrocatalytic oxygen evolution reactions [59]. The coupling of DTM MXenes can improve the conductivity and reduce charge transfer resistance. The doped composite has revealed excellent efficiency with low overpotential (410 mV @ 200 mA/cm²). This strategy and heterostructure engineering could develop on electrocatalytic water splitting.

According to Jin and colleagues' study [60] on 24 double-transition metal carbides including $M_2M'C_2T_x$ and $M_2M_2'C_3T_x$, it is predicted that 18 MXenes are active electrocatalysts to HER. In particular, $Nb_2Ta_2C_3$, $Ti_2M_x'C_y$, and $Mo_2M_x'C_y$ with O-termination are the most stable carbides under standard conditions, while O- and OH-terminated $V_2M_2''C_3$ and $Cr_2M_x''C_y$ are the most stable carbides. As a guide remark, the more fragile the M–O bonds of carbides, the stronger the bond between the adsorbed hydrogen and the terminal -O group. Furthermore, Geng et al. [32] have found that ΔG_H values of $M_2M''C_2T_x$ (T: O and N) monolayers are very negative and also hold very low exchange current. The weak interaction in S–Cr₂TiC₂, S–Cr₂VC₂, and P–Mo₂TiC₂ boosts the H₂ release and causes to very increased exchange current which is useful for H₂ evolution reaction.

4.2. Batteries

For the first time, Mashtalir et al. [61] used MXenes as anodes in lithium batteries and found their excellent charging capacity. The electrochemical intercalations of lithium between carbonitride nanosheets conduct 2D MXenes as favorable solids to construct anodes in Li-ion batteries and capacitors. Not long after, the performance of $Ti_3C_2T_x$ MXene in energy storage was successfully extended by lithium/sodium [62]. However, the limited practical capacity and the tendency of MXenes to accumulate during the electrochemical cycle reduce the efficiency of lithium batteries [63]. DTM carbonitrides are admiringly suitable as an anode in batteries because of their excellent capacity in comparison with conventional single-metal carbonitrides.

Based on the stability of DTM MXenes, MoWC, and MoWCO₂ have been chosen by Zhou et al. as the anode in the Na battery in order to store energy [64]. Because the distinct radii of the metal atoms lead to the crystalline lattice of ordered DTM carbonitrides [8], MXenes with excellent properties are formed based on surface engineering, which is suitable for electrode preparation. The molybdenum and tungsten have different radii that could synthesize ordered W–C–Mo MXenes in a large area. The synergy of Mo and W leads to the high capacity of this type of MXenes, and the oxygen functional group does not change it. According to a previous study on W₂C MXene [65], more electrons gathered on the surface of MoWC which leads to a high charge state. It should be mentioned that there are very small diffusion barriers in sodium batteries like lithium batteries [66], which is incompatible with diffusion barriers in Mo₂C [67] and W₂C [65] monolayers. In addition, MoWC monolayers have a high specific capacity of about 670 mAh/g as anode materials for lithium batteries [66]. Moreover, WCrC and WCrCO₂ with superior dynamical stability are known as ideal anode materials with ignoble diffusion barriers for the development of sodium-ion batteries [68].

In theoretical research, Li et al. [69] studied the terminated functional group effect on the TiNbC behavior. They found that the -OH group destabilizes TiNbC(OH)2 although it has metallic conductivity. Furthermore, fluorine groups make TiNbCT2 undesirable as an anode material because of the forming of lithium-ion rings. In particular, TiNbC and TiNbCO₂ MXenes show distinctive features such as very low lithium diffusion barriers, theoretical storage capacity, and moderate absorption energy comparable to Ti₂C [70] and Nb₂C [71] monolayers, which manifests bimetallic TiNbC and TiNbCO2 are suitable for Li-ion batteries with capacity of 350 and 290 mAhg-1, respectively. In another research, it has been determined that TiNbC and TiNbCO₂ have a higher ability than Nb₂C-based single-transition metal MXenes to absorb sodium atoms in a Na-ion battery, which is attributed to the synergistic effect of titanium and niobium, which causes the interaction between the substrate and sodium [72]. In another work, Liu and coworkers [73] have successfully fabricated $Ti_2NbC_2T_x$ as a double transition metal MXene with enlarged interlayer spacing. This anodic material provides fast charge transfer and ion diffusion with a fine capacity of 196 mAh/g which is guite stable during more than 400 cycles.

Previously, the hybridization of single metal MXenes with metallic oxide has been investigated for energy storage in batteries [74]. Therefore, the bimetallic MXenes composite based on metal oxide has been considered. In the studies of Dai et al., (Ti_{0.9}Nb_{0.1})₃C₂ has shown a specific capacity of 280 mAh/g at a current density of 0.1 A/g and retains 91.5% of its capacity after 2000 cycles [75]. Hence, the Nb-TiO₂/(Ti_{0.9}Nb_{0.1})₃C₂ nanohybrid architecture through an annealing approach leads to a high-performance and stable anode material due to reversible and fast Li ions diffusion and storage with Nb-TiO₂ support. As mentioned, to overcome the unstable structure and limited capacity of 2D MXene, Niobium-doped TiO2 can be a good choice for anode materials in batteries [40]. In this regard, Nb-doped TiO₂/TiNbC nanolayers prevent structural collapse and reassembly during charge and discharge and promote space Li ions transportation. However, compared to Nb-TiO₂/(Ti_{0.9}Nb_{0.1})₃C₂, it has shown a lower reversible performance (260 mAh/g) after 500 cycles. Although TiO₂ is the most widely used semiconductor for the fabrication of hybrid anodic materials, Xu et al. [76] have chosen VNbO5 metallic oxide over VNbCT_x. The specific capacity of VNbO₅/VNbCT_x is greatly improved compared to V₂O₅ for energy storage in lithium batteries (400 mAh/g> 294 mAh/g). At the same time, other researchers have made a novel 211-phase VNbCT_x by selectively etching the aluminum layer of VNbAlC, which shows a specific capacity of 520 mAh/g with hopeful



Fig. 10. a) Rate performance of VNbCTx electrode at different current densities, b) CV curves of VNbCTx electrode at a scan rate of 1 mV/s with calculated capacitive-controlled contribution in the shaded region, and c) bar graph depicting capacitive-controlled and diffusioncontrolled current contribution at different scan rate.

cycle stability and high rate capability in Li batteries as shown in Fig. 10 [77]. The superior performance is related to the multilayer skeleton of VNbCT_x MXene which can prevent the restacking of mono metal MXene nanosheets. In addition to VNbO₅, TiNbO_x is also hybridized as a mixed metal oxide with carbides to obtain a combination with versatile structural and electrochemical properties. For example, Husmann and coworkers [42] have designed and prepared a TiNb-based carbide/TiNbO_x hybrid via thermal oxidation in CO₂ to test as a Li-ion battery electrode. The TiNbO_x/TiNbC presented a high 226 mAh/g capacity at 10 mA/g and 75% retention after 1000 cycles at 1 A/g with Nb/Ti: 5 in derived TiNbO_x.

Previously, ordered and functionalized TiVC has been investigated through density functional theory calculations and is a candidate anode material for Li-ion batteries [78]. Although all the samples have high electronic conductivity and show metallic characteristics, TiVCT₂ functionalized with the sulfur group has shown the lowest barrier to the diffusion of a Li-ion. In addition, in the charge/discharge process, the formation of alkali metal dendrites is prevented by the range of open circuit voltage of lithium ions (0.0-1.0 V) with monolayers of pristine TiVC and TiVCS₂. In another work, both ordered and solid-solution structures of TiVC and TiVCT₂ have been analyzed as lithium-ion anode materials [79]. In comparison, ordered and solid types of TiVC exhibited excellent adsorptive properties, and the lowest diffusion barriers belong to two different sides of ordered TiVC with the highest theoretical capacity ~480 mAh/g. It is noteworthy that the decreasing trend of TiVC capacity has been observed when it is functionalized with -O, -F, and -OH, respectively. Furthermore, functionalized $TiVCT_x$ blended V_2O_5 and TiO_2 as anode material boosts the Li-ion batteries' performance to 331 mAh/g [80]. In another study, a 3D TiVCT_x/poly-o-phenylenediamine composite has been proposed as a chemical and electrochemical stable electrode material in Li-ion batteries [81]. This tremella-like architecture composite has exhibited outstanding properties with a capacity of up to 224 mAh/g at 2 A/g. Compared to the V₄C₃T_x/poly-o-phenylenediamine with a capacity of 561 mAh/g at 0.1 A/g [82], the blend of MXenes and conductive polymers is recommended as electrode material. In addition, the TiO₂based heterostructure of TiVCT_x is a promising strategy for highperformance anode materials [83]. Ti atoms of Ti_{2-v}V_vCT_x could be selectively oxidized on titania particles while V atoms maintain the two-dimensional lamella structure with elevated electronic conductivity. The calculated capacitance contribution is 64% when the scan speed reaches 1 mV/s (Fig. 11). This indicates that the quasicapacitor control contribution to the total capacity is dominant, which is associated with fast Li⁺ storage and superior rate performance.

According to the theory of Tan and coworkers [84], the molybdenum atom prefers to occupy the surface layer in $(M_{1-x}Mo_x)_3C_2$ (where M is Nb, V, Ti, or Ta) and based on Monte Carlo simulation, the ordering continues up to the above temperature. In this regard, Huang and collogues [85] have shown that TiMoC monolayers have low Li-ion diffusion barriers on the titanium surface. Moreover, if chromium is substituted for molybdenum and the concentration of lithium is increased to 2, the theoretical capacity will be 480 mAh/g. In addition, TiCrCO₂ displayed a somewhat elevated theoretical capacity of ~370 mAh/g. Therefore, TiCrC, TiMoC, and TiCrCO₂ monolayers can be good candidates for the anode material in lithium batteries. Fundamentally, the surface terminations influence the Li-ion adsorption and the theoretical capacity of Mo-based MXenes [86]. Except for –O and –H terminations, it is predicted fast



Fig. 11. a) Capacitance contribution of $TiO_2/Ti_{2-y}V_yCT_x$ (1:1) at different scan rates and b) charge/discharge galvanostatic intermittent titration technique curves of $TiO_2/Ti_{2-y}V_yCT_x$ and corresponding lithium ions diffusion coefficient.

charging/discharging process and low barriers of lithium ions (\sim 0.04 eV) for Mo-based MXenes including V, Ti, and Sc.

The main obstacle to large-scale energy storage and conversion systems is the lack of cost-effective, stable, and efficient catalysts. In this regard, NbTaC, VTaC, and VNbC have been designed as double transition metal MXenes with a functionalized terminal to increase anode performance in Na ions batteries [87]. Compared to the single metal counterpart, the Na⁺ absorption capacity of NbTaC, VTaC, and VNbC enhances to 75, 37, and 75%, respectively. These composites not only have low initial migration barriers with sodium atoms, but also have high theoretical capacity (NbTaC: 328, VTaC: 302, and VNbC: 602 mAh/g). In another study, (Nb_yV_{2-y})CT_x solid-solution MXene has been explored for energy storage in Li-ion batteries [47]. In lithium-ion batteries, the electrochemical cycling of Nb_yV_{2-y}C-derived oxides displayed differing behaviors to V₂C anodes [88].

Of course, single and double layers of nitride-based transition metal containing vanadium and chromium have a bright future in lithium-ion batteries. For example, V2N and VCrN monolayers have a low energy diffusion barrier of 0.034 and 0.03 eV in Li-ion batteries, respectively [89]. Adsorption of Li-ion multilayers on the upper and lower V₂N/CrVN in a specific capacity surfaces results of 1440.0/1040.0 mAh/g. Further, both mentioned MXenes are thermally stable at 27 and 227 °C. In addition, thallium in DTM Ti-based MXenes has been used as a Li-ion host anode with a remarkable capacity of 460 mAh/g and kept efficiency of around 99% after 200 cycles [90] The great Li-ion storage of the bimetallic $Ti_x Ta_{(4-x)}C_3T_x$ could be correlated to the formation of a stable bi-metallic MXene structure, which stores Li-ions on the surface of its layers during the redox reaction. The $Ti_xTa_{(4-x)}C_3T_x$ demonstrated good electronic conductivity between the active materials, carbon additive, and binder, showing good electrochemical properties, remarkable capacity, and great capability [91].

4.3. Magnetic nanodevices

Double transition metal MXenes have semi-metallic properties and intrinsic magnetism that can be used in magnetic and spintronic devices. MXenes research is rapidly evolving to on the application in magnetic devices [92]. Magnetic tunnel junctions called spintronics as nanostructured tools consist of two layers of magnetic metal separated by an ultrathin layer of insulator [93]. These implements are used in the fabrication of magnetic sensors, hard disk drives, magnetic random access memories, etc. [94].

Recently, Cui et al. [95] have employed $ScCr_2C_2F_2$ as the spin-filter tunnel barrier to achieve excellent spin-filtering in the van der Waals magnetic tunnel junction. It has been observed that the $ScCr_2C_2F_2$ monolayers can preserve half-metallicity with good polarization after utilization in magnetic devices. Other Cr-based MXenes, emerging $Mo_2CrN_2O_2$ and $W_2CrN_2O_2$ with varying metallic behaviors and robust ferromagnetism have great potential in electronic devices and nanospintronics [28]. The direct bandgap of $Mo_2CrN_2O_2$ and $W_2CrN_2O_2$ are 0.77 and 1.35 eV opening up an optimistic future in the preparation of new 2D materials with adjustable magnetic features. It is notable that the bandgap of semiconductors can be predicted using density functional theory (typical errors are <0.1 eV) [96].

A wide group of ordered DTM MXenes such as Ti-V, Ti-Cr, and Ti-Mn with central Ti layers and various terminal groups have been explored by Sun et al. [55]. It has been found that F-terminated TiMn₂N₂ has a unique wide bandgap of up to 1.0 eV while the unfunctionalized TiMn₂N₂ remains metallic. Therefore, by using wide combinations of bimetallic MXenes, new magnetic, semi-metallic, or insulating behaviors can be achieved with or without surface terminations. Moreover, the magnetic and electronic properties of functionalized M2M'C2Tx MXenes (T: S, P, O, N, and B) have been investigated by DFT for use in nanodevices [32]. Based on the stability, a set of DTM MXenes has been screened including Cr₂VC₂T_x, Cr₂TiC₂T_x, and Mo₂VC₂T_x (T: S, O, and N), which are spontaneously conductive. The magnetic moments of Cr₂M'C₂T_x (M: V and Ti, T: S, O, and N) are mainly contributed by Cr atoms. Differently, S-Cr2M'C2 (M': Ti and V) monolayers are antiferromagnetic, while Mo₂VC₂T_x (T: S, O, and N) maintain ferromagnetism at ground state with magnetic moment localized on vanadium. These functionalized DTM carbonitrides are favorable composites for magnetic nanodevices

In another work, Ti₂MnC₂T₂ monolayers have been introduced as strong ferromagnetism regardless of surface terminations (T: F, OH, and O) for nanoscale spintronic applications [97]. Both O-terminated Hf₂VC₂ and Hf₂MnC₂ MXenes as 2D robust ferromagnetic materials have high magnetic moments as well as great Curie temperatures based on electron filling in transition-metal cations. Furthermore, Hantanasirisakul et al. [98] have reported comprehensive studies on magnetic as well as electronic properties of TiCr₂C₂T_x MXene for potential spintronic applications. It has been found that a magnetic transition is present in $TiCr_2C_2T_x$ @ around 30 K, which does not exist in its bulk-nanolayered counterpart (TiCr₂AlC₂). Besides the Cr cation, the magnetic behavior of the Nb-based 2D MXenes can be observed [99]. For instance, the magnetization of solid solution (Nb_{1-x}Ti_x)₄C₃ MXene emerges driven by Ti atoms on the surfaces. In addition, the magnetic features of the mentioned MXene are preserved upon the surface functionalization by OH or F groups. In addition to carbide MXenes, the nitride family has also been proposed for use in electronic devices. WSi₂N₄ and MoSi₂N₄, emerging 2D semiconductors, have practical potential for designing energy-efficient and high-performance composites [100, 101].

4.4. Antibacterial

Most of the applications of composites are focused on energy production [102]. Recently, 2D MXenes have been used in biomedical scopes and antibacterial due to their great bio-compatibility and photothermal properties. [103]. To overcome bacterial infections and antibiotic resistance, $TiVCT_x$ monolayers have been synthesized and demonstrated their dual-functional antibacterial ability [104]. The Ti-V MXene has exhibited a usual lamellar structure and it also demonstrated above 99.8% antibacterial ability against B. subtilis and E. coli after exposure to low-dose carbide. In addition, the photothermal effect of Ti-V carbide has been examined by NIR laser. Such a double metal MXene showed a stable temperature under 3 times on and off irradiation cycle (Fig. 12), indicating outstanding photothermal stability of $TiVCT_x$.

4.5. Chemical synthesis

One of the crises of the last century is providing affordable energy from renewable sources [105]. Hydrogenation of CO and CO₂ on metal carbide or nitride-based composites is growing as a two-dimensional platform as a substitute for noble metal catalysts to achieve green fuels via various processes [106]. In this regard, Mo, W carbide, and nitride have been used by Patterson et al. [107] as single metal MXene for the Fischer-Tropsch reaction to produce methane as hydrocarbon products in a stirred reactor. Other monometallic MXenes families such as TiC [108] and Nb₂C [109] have been used to reduce CO₂ and methanol production. It has been proven that the lack of functional groups on the surface of molybdenum carbide has a positive effect on the selectivity and activity of MXene [110]. This conclusion cannot be taken in the case of DTM MXenes because the properties and behavior of the bimetallic species are very different. Recently, Wu and his colleagues [111] have effort to reduce the greenhouse gas CO₂ by Ru-Mo₂TiC₂ as a prominent sunlight absorber with a rate of 4 mol/g_{Ru}.h CO production which is 2.5 and 80 times higher than Ru clusters and Ru/SiO₂. Mo-based nitrides have also high potential to be a

good composite in the field of photocatalysis [112]. For example, $MoSi_2N_4$ hybridized with $MoSiGeN_4$ has been suggested for photocatalytic CO_2 reduction due to the suitable bandgap of energy.

The commercial conversion of N_2 to urea by CO_2 through the Wöhler synthesis [113] is used to promote energy and environmental strategies. Global urea and ammonia production account above 2% of the world's energy consumption. Therefore, it is necessary to produce urea with high-performance electrocatalysts under moderate conditions. However, the common process suffers from many technical bottlenecks to proceed under mild conditions. In new research, for the first time, Yang and co-workers [114] designed Mo₂VC₂ DTM carbide as a promising electrocatalyst for urea synthesis. Although Mo₂VC₂ has a lower potential than the Cu-Pd catalyst [115], it has opened a bright horizon for nitrogen-to-urea conversion.

Improving the Haber-Bosch process for NH3 generation via N2 reduction can reduce greenhouse gas emissions [116]. DFT calculations can screen the effective metal atoms as supporting defective Mo₂TiC₂O₂ nanosheets, which significantly promote the N₂ reduction reactions. Recently, doping of Mo2TiC2O2 with Zr single atoms has been explored for nitrogen reduction at ambient conditions [117]. The formation energy of Zr-doped Mo2TiC2O2 is more negative than synthesized Pt-doped Mo₂TiC₂O₂, which indicates the readiness of this composite to be a good candidate for N2 conversion. It should be noted that in the process of nitrogen reduction, the lowest barrier of the potential determination stage is reported to be 0.15 eV. It has been proved that N2 molecules could intensely adsorb on DTM carbides and activate for NH₃ production. Another DTM MXene candidate is Mo₂Nb₂C₃ with a low overpotential of 0.48 V [118]. Among the 18 MXenes shown in Fig. 13, Mo₂Nb₂C₃ has the lowest reaction-free energy of the potential determining step (ΔG_{PDS}). Molybdenum molecules can control the electrons required for the reaction and increase the activity of the N2 fixation. Combining DFT calculations and Monte Carlo simulation, Fang and his coworkers [119] have introduced 5 potential DTM MXenes consisting of V-Mo, Nb-Cr, Mo-Mn, and Mo-W for N2 reduction reaction.



Fig. 12. Photothermal stability of the $TiVCT_x$ under laser irradiation (0.1 W/cm², 808 nm, and 40 µg/ ml) for 5 min and operated by turning the laser on and off for 3 cycles.



Fig. 13. ΔG_{PDS} for some type of DTM MXenes (color codes represent the corresponding PDS of each step). ΔG_{PDS} for all DTM carbides are below 0.8 eV.

4.6. Sensors and biosensors

The chemical composition and layered structure, and high conductivity of MXenes have made them attractive for the application and development of sensors and biosensors [120]. In addition, 2D MXenes display suitable bandgap, lower current leakage and low diffusion barriers, thereby improving detection sensitivity [121]. Therefore, gas sensors based on MXenes, electrochemical and optical biosensors have been studied and researched. In one case, 2D MoSi₂N₄ monolayers have been studied as sensors for, SO2, NO, NO2, and O2 detection [122]. It has been found that the surface of MoSi₂N₄ acts as a charge acceptor or donor and all molecules are physically adsorbed on the surface by small charge transfer. With the physisorbtion of gas molecules, the semiconducting property of MoSi₂N₄ does not change and the bandgap distance decreases from 1.79 to 1.50 eV. Later, sensing of sulfur-containing gases (SO2 and H₂S) on M₂TiC₂T_x (M: Cr, Mo; T_x: O, OH, S) layers have been investigated by means of DFT calculation [123]. The physisorbtion of SO2 is stronger on S-terminated Mo2TiC2 and Cr_2TiC_2 , whereas H_2S has higher adsorption on 0functionalized Mo₂TiC₂ and Cr₂TiC₂ (Fig. 14a). The isobaric surface coverage of SO2 and H2S vs. temperature is shown in Fig. 14b. As can be clearly seen in the figure, Cr₂TiC₂O₂ and MoTiC₂O₂ are able to detect toxic gases containing very dilute

sulfur. In another research, Xu et al. [124] investigated the effect of noble metals absorbed on MoSi2N4 in the field of gas sensor construction and nitrogen oxide removal. They found that Au-based MoSi₂N₄ is suitable for sensing O₂, CO, and SO₂ gas molecules, while Pd-based MoSi₂N₄ is more capable of detecting NO2, NO, and N2 gases, and Ag-based MoSi2N4 is only useful for SO₂ sensing. Furthermore, the introduction of Pd atoms on MoSi₂N₄ increases the photocatalytic ability of NO removal and prevents the disposal of the toxic NO2 product because the noble metal atoms reduce the bandgap and improve the ability to absorb light. For the first time, Linghu et al. [125] have proposed Cu-MoSi₂N₄ monolayers for the adsorption of NH3 molecules. The process performance has been analyzed via both non-equilibrium Green's function and DFT. The results of electronic transport calculations have shown that although this composite is sensitive to NH₃, CO, NO, and NO₂ gases, it only moderately adsorbs NH3 at RT.

In a recent study, SnS₂ and Mo₂TiC₂ quantum dots (QDs) have been designed for a novel electrochemiluminescence biosensor to detect gastric cancer [126]. MoTi-MXene quantum dots have a substantial contribution to the luminescence procedure due to their stability and light processing [127]. SnS₂ nanolayers also increase the brightness intensity of MXenes quantum dots due to their large surface area and low dielectric constant [128, 129]. Therefore, SnS₂/Mo₂TiC₂ QDs is a good candidate for biosensor application.



Fig. 14. a) The adsorption energy of H₂S and SO₂ molecules with Mo₂TiC₂S₂, Mo₂TiC₂O₂, Cr₂TiC₂S₂, and Cr₂TiC₂O₂ layers and b, c) isobaric surface coverages of SO₂ and H₂S with mentioned MXenes at various temperatures.

5. Conclusions

The selection of metals with a useful hybrid effect has opened new ways for potential applications with desirable properties in the MXenes family. However, the low investigation of physical, mechanical, and electronic characteristics has limited their practical application. The behavior of DTM MXenes is different from single metal MXenes, which can have various uses in the future. This group of twodimensional materials has greatly helped in designing nanomaterials and meeting new needs. Knowing the electrochemical, metallic, and semiconducting properties of DTM MXenes can ultimately lead to understanding their performance in various applications. Thermodynamic stability is the very first property of the DTM MXenes which is discussed with the role of terminal groups. Most of the MXenes studied have shown metallic properties, thus providing superior charge transport. However, the synthesis of DTM MXenes as newly interesting discovered materials still requires more theoretical and experimental knowledge about characteristics and capabilities.

These results indicate the wide application of bimetallic MXenes from the electrocatalytic production of hydrogen to the anode material in batteries and electronic devices, etc. Various methods have been proposed for the synthesis and preparation of MXenes. Furthermore, the development of new applications is provided with the possibility of structural modification.

CRediT authorship contribution statement

Asieh Akhoondi: Writing – original draft, Resources, Supervision. Mitra Ebrahimi Nejad: Writing – review & editing. Mohammad Yusuf: Writing – review & editing. Tejraj M. Aminabhavi: Writing – review & editing. Khalid Mujasam Batoo: Writing – review & editing. Sami Rtimi: Writing – review & editing.

Data availability

As this is a review article, no new data were generated. All information is publicly available or cited appropriately within the article.

Declaration of competing interest

This research received no external funding. The authors have no acknowledgments to declare.

Funding and acknowledgment

This research received no external funding.

References

- S. Kanungo, G. Ahmad, P. Sahatiya, A. Mukhopadhyay, S. Chattopadhyay, 2D materials-based nanoscale tunneling field effect transistors: current developments and future prospects, npj 2D Mater. Appl. 6 (2022) 83. https://doi.org/10.1038/s41699-022-00352-2.
- [2] D. Er, K. Ghatak, Atomistic modeling by density functional theory of two-dimensional materials, Micro and Nano Technologies, Elseviear. (2020) 113–123. https://doi.org/10.1016/B978-0-12-818475-2.00006-4.
- [3] V. Shanmugam, R.A. Mensah, K. Babu, S. Gawusu, A. Chanda, et al., A Review of the Synthesis, Properties, and Applications of 2D

Materials, Part. Part. Syst. Charact. 39 (2022) 2200031. https://doi.org/10.1002/ppsc.202200031.

- [4] Z. Xiong, L. Zhong, H. Wang, X. Li, Structural Defects, Mechanical Behaviors, and Properties of Two-Dimensional Materials, Materials. 45 (2021) 1192. https://doi.org/10.3390/ma14051192.
- [5] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, et al., Two-Dimensional Nanocrystals Produced by Exfoliation of Ti3AlC2, Adv. Matter. 23 (2011) 4248–4253. https://doi.org/10.1002/adma.201102306.
- [6] M. Kurtoglu, M. Naguib, Y. Gogotsi, M.W. Barsoum, First principles study of two-dimensional early transition metal carbides, MRS Commun. 2 (2012) 133–137. https://doi.org/10.1557/mrc.2012.25.
- [7] M. Naguib, V.N. Mochalin, M.W. Barsoum, Y. Gogotsi, MXenes: a new family of two-dimensional materials, Adv. Mater. 26 (2014) 992–1005. https://doi.org/10.1002/adma.201304138.
- [8] B. Anasori, Y. Xie, M. Beidaghi, J. Lu, B.C. Hosler, et al., Two-Dimensional, Ordered, Double Transition Metals Carbides (MXenes), ACS Nano. 9 (2015) 9507–9516. https://doi.org/10.1021/acsnano.5b03591.
- [9] M. Tawalbeh, S. Mohammed, A. Al-Othman, M. Yusuf, M. Mofijur, H. Kamyab, MXenes and MXene-based materials for removal of pharmaceutical compounds from wastewater: Critical review, Environ. Res. 228 (2023) 115919. https://doi.org/10.1016/j.envres.2023.115919.
- [10] Y. Cheng, J. Dai, Y. Zhang, Y. Song, Two-Dimensional, Ordered, Double Transition Metal Carbides (MXenes): A New Family of Promising Catalysts for the Hydrogen Evolution Reaction, J. Phys. Chem. C. 122 (2018) 28113–28122. https://doi.org/10.1021/acs.jpcc.8b08914.
- [11] M. Zhu, C. Lu, L. Liu, Progress and challenges of emerging MXene based materials for thermoelectric applications, iScience. 26 (2023) 106718. https://doi.org/10.1016/j.isci.2023.106718.
- [12] C. Zhang, Y. Zhang, X. Gu, C. Ma, Y. Wang, et al., Radiation synthesis of MXene/Ag nanoparticle hybrids for efficient photothermal conversion of polyurethane films, RSC Adv. 13 (2023) 15157–15164. https://doi.org/10.1039/d3ra02799f.
- [13] A. Akhoondi, M. Mirzaei, M.Y. Nassar, Z. Sabaghian, F. Hatami, M. Yusuf, New strategies in the preparation of binary g-C3N4/MXene composites for visible-light-driven photocatalytic applications, Synth. Sinter. 2 (2022) 151–169. https://doi.org/10.53063/synsint.2022.24121.
- [14] M. Naguib, J. Halim, J. Lu, K.M. Cook, L. Hultman, et al., New twodimensional niobium and vanadium carbides as promising materials for Li-ion batteries, J. Am. Chem. Soc. 135 (2013) 15966–15969. https://doi.org/10.1021/ja405735d.
- [15] M. Feng, W. Wang, Z. Hu, C. Fan, X. Zhao, et al., Engineering chemical-bonded Ti3C2 MXene@carbon composite films with 3D transportation channels for promoting lithium-ion storage in hybrid capacitors, Sci. China Mater. 66 (2023) 944–954. https://doi.org/10.1007/s40843-022-2268-9.
- [16] A. Akhoondi, H. Ghaebi, L. Karuppasamy, M.M. Rahman, P. Sathishkumar, Recent advances in hydrogen production using MXenes-based metal sulfide photocatalysts, Synth. Sinter. 2 (2022) 37–54. https://doi.org/10.53063/synsint.2022.21106.
- [17] L. Chen, X. Dai, W. Feng, Y. Chen, Biomedical Applications of MXenes: From Nanomedicine to Biomaterials, Acc. Mater. Res. 3 (2022) 785–798. https://doi.org/10.1021/accountsmr.2c00025.
- [18] H. Bark, G. Thangavel, R.J. Liu, D.H.C. Chua, P.S. Lee, Effective Surface Modification of 2D MXene toward Thermal Energy Conversion and Management, Small Methods. 7 (2023) 2300077. https://doi.org/10.1002/smtd.202300077.
- [19] W. Hong, B.C. Wyatt, S.K. Nemani, B. Anasori, Double transitionmetal MXenes: Atomistic design of two-dimensional carbides and nitrides, MRS Bull. 45 (2020) 850–861. https://doi.org/10.1557/mrs.2020.251.

- [20] Z.W. Seh, K.D. Fredrickson, B. Anasori, J. Kibsgaard, A.L. Strickler, et al., Two-Dimensional Molybdenum Carbide (MXene) as an Efficient Electrocatalyst for Hydrogen Evolution, ACS Energy Lett. 1 (2016) 589–594. https://doi.org/10.1021/acsenergylett.6b00247.
- [21] M.G. Moreno-Armenta, J. Guerrero-Sánchez, S.J. Gutiérrez-Ojeda, H.N. Fernández-Escamilla, D.M. Hoat, R. Ponce-Pérez, Theoretical investigation of the MXene precursors MoxV4-xAlC3 (0 ≤ x ≤ 4), Sci. Rep. 13 (2023) 3271. https://doi.org/10.1038/s41598-023-30443-z.
- [22] A.P. Umanskii, V.A. Lavrenko, S.S. Chuprov, V.P. Konoval, Hightemperature oxidation of composites based on titanium carbonitride and double titanium-chromium carbide, Refract. Ind. Ceram. 47 (2006) 246–250. https://doi.org/10.1007/s11148-006-0099-5.
- [23] S. Venkateshalu, G.M. Tomboc, B. Kim, J. Li, K. Lee, Ordered Double Transition Metal MXenes, ChemNanoMat. 8 (2022) e202200320. https://doi.org/10.1002/cnma.202200320.
- [24] E. Omugbe, O.E. Osafile, O.N. Nenuwe, E.A. Enaibe, E.E. Elemike, Thermal and electrical transport conductivities of novel ordered double two-dimensional MXenes via density functional theory, Can. J. Chem. 101 (2023) 316–325. https://doi.org/10.1139/cjc-2022-0070.
- [25] W.-L. Chang, Z.-Q. Sun, Z.-M. Zhang, X.-P. Wei, X. Tao, Thermoelectric properties of two-dimensional double transition metal MXenes: ScYCT2 (T=F, OH), J. Phys. Chem. Solids. 176 (2023) 111210. https://doi.org/10.1016/j.jpcs.2022.111210.
- [26] N.M. Caffrey, Prediction of Optimal Synthesis Conditions for the Formation of Ordered Double-Transition-Metal MXenes (o-MXenes), J. Phys. Chem. C. 124 (2020) 18797–18804. https://doi.org/10.1021/acs.jpcc.0c05348.
- [27] E. Bolen, E. Deligoz, Computational study of mechanical stability and phonon properties of MXenes Mo2ScC2T2 (T = O and F): 2D materials, J. Appl. Phys. 130 (2021) 065102. https://doi.org/10.1063/5.0055701.
- [28] K.D. Dihingia, S. Saikia, N. Yedukondalu, S. Saha, S.G. Narahari, 2D-Double transition metal MXenes for spintronics applications: surface functionalization induced ferromagnetic half-metallic complexes, J. Mater. Chem. C. 10 (2022) 17886–17898. https://doi.org/10.1039/D2TC03067E.
- [29] E.M.D. Siriwardane, P. Karki, Y.L. Loh, D. Çakır, Engineering magnetic anisotropy and exchange couplings in double transition metal MXenes via surface defects, J. Phys: Condens. Matter. 33 (2021) 035801. https://doi.org/10.1088/1361-648X/abba8e.
- [30] Y. Zhang, C. Zhou, B. Sa, N. Miao, J. Zhou, Z. Sun, Computational design of double transition metal MXenes with intrinsic magnetic properties, Nanoscale Horiz. 7 (2022) 276–287. https://doi.org/10.1039/D1NH00621E.
- [31] X. Jiang, A.V. Kuklin, A. Baev, Y. Ge, H. Ågren, et al., Twodimensional MXenes: From morphological to optical, electric, and magnetic properties and applications, Phys. Rep. 848 (2020) 1–58. https://doi.org/10.1016/j.physrep.2019.12.006.
- [32] J. Geng, R. Wu, H. Bai, I.-N. Chan, K.W. Ng, et al., Design of functionalized double-metal MXenes (M2M³C2T2: M = Cr, Mo, M³ = Ti, V) for magnetic and catalytic applications, Int. J. Hydrog. Energy. 47 (2022) 18725–18737. https://doi.org/10.1016/j.ijhydene.2022.04.058.
- [33] D.R. Kumar, R. Karthik, M. Hasan, M.S. Sayed, J.-J. Shim, Mo-MXene-filled gel polymer electrolyte for high-performance quasisolid-state zinc metal batteries, Chem. Eng. J. 473 (2023) 145207. https://doi.org/10.1016/j.cej.2023.145207.
- [34] B.C. Wyatt, A. Thakur, K. Nykiel, Z.D. Hood, S.P. Adhikari, et al., Design of Atomic Ordering in Mo2Nb2C3Tx MXenes for Hydrogen Evolution Electrocatalysis, Nano Lett. 23 (2023) 931–938. https://doi.org/10.1021/acs.nanolett.2c04287.
- [35] K.R.G. Lim, M. Shekhirev, B.C. Wyatt, B. Anasori, Y. Gogotsi, Z. W. Seh, Fundamentals of MXene synthesis, Nat. Synth. 1 (2022) 601–614. https://doi.org/10.1038/s44160-022-00104-6.
- [36] Y. Gogotsi, B. Anasori, The Rise of MXenes, ACS Nano. 13 (2019) 8491–8494. https://doi.org/10.1021/acsnano.9b06394.

121

- [37] S.A. Zahra, M.W. Hakim, M.A. Mansoor, S. Rizwan, Twodimensional double transition metal carbides as superior bifunctional electrocatalysts for overall water splitting, Electrochim. Acta. 434 (2022) 141257. https://doi.org/10.1016/j.electacta.2022.141257.
- [38] K. Byrappa, T. Adschiri, Hydrothermal technology for nanotechnology, Prog. Cryst. Growth Charact. Mater. 53 (2007) 117–166. https://doi.org/10.1016/j.pcrysgrow.2007.04.001.
- [39] A. Akhoondi, M. Aghaziarati, N. Khandan, Production of highly pure iron disulfide nanoparticles using hydrothermal synthesis method, Appl. Nanosci. 3 (2013) 417–422. https://doi.org/10.1007/s13204-012-0153-1.
- [40] Q. Ma, Z. Zhang, P. Kou, D. Wang, Z. Wang, et al., In-situ synthesis of niobium-doped TiO2 nanosheet arrays on double transition metal MXene (TiNbCTx) as stable anode material for lithium-ion batteries, J. Colloid Interface Sci. 617 (2022) 147–155. https://doi.org/10.1016/j.jcis.2022.03.007.
- [41] K. Byrappa, N. Keerthiraj, S.M. Byrappa, Hydrothermal Growth of Crystals—Design and Processing, Handbook of Crystal Growth (Second Edition), Elsevier. (2015) 535–575. https://doi.org/10.1016/B978-0-444-63303-3.00014-6.
- [42] S. Husmann, M. Besch, B. Ying, A. Tabassum, M. Naguib, V. Presser, Nb Carbides (MXene) as Anode Materials for Li-Ion Batteries, ACS Appl. Energy Mater. 5 (2022) 8132–8142. https://doi.org/10.1021/acsaem.2c00676.
- [43] A. Akhoondi, Z. Mahmoud, Khandan Nahid, Hydrothermal Production of Highly Pure Nano Pyrite in a Stirred Reactor, Iran. J. Chem. Chem. Eng. 33 (2014) 15–19. https://doi.org/10.30492/IJCCE.2014.7189.
- [44] Y.-T. Liu, P. Zhang, N. Sun, B. Anasori, Q. Zhu, et al., Self-Assembly of Transition Metal Oxide Nanostructures on MXene Nanosheets for Fast and Stable Lithium Storage, Adv. Mater. 30 (2018) 1707334. https://doi.org/10.1002/adma.201707334.
- [45] C. Zhang, S.J. Kim, M. Ghidiu, M.Q. Zhao, M.W. Barsoum, et al., Layered Orthorhombic Nb2O5@Nb4C3Tx and TiO2@Ti3C2Tx Hierarchical Composites for High Performance Li-ion Batteries, Adv. Funct. Mater. 26 (2016) 4143–4151. https://doi.org/10.1002/adfm.201600682.
- [46]M. Fides, P. Hvizdoš, R. Bystrický, A. Kovalčíková, R. Sedlák, et al., Microstructure, fracture, electrical properties and machinability of SiC-TiNbC composites, J. Eur. Ceram. Soc. 37 (2017) 4315–4322. https://doi.org/10.1016/j.jeurceramsoc.2017.05.004.
- [47] M.A. Andrade, T. Averianov, C.E. Shuck, K. Shevchuk, Y. Gogotsi, E. Pomerantseva, Synthesis of 2D Solid-Solution (NbyV2–y)CTx MXenes and Their Transformation into Oxides for Energy Storage, ACS Appl. Nano Mater. 6 (2023) 16168–16178. https://doi.org/10.1021/acsanm.3c02004.
- [48] J. Zhang, Y. Zhao, X. Guo, C. Chen, C.-L. Dong, et al., Single platinum atoms immobilized on an MXene as an efficient catalyst for the hydrogen evolution reaction, Nat. Catal. 1 (2018) 985–992. https://doi.org/10.1038/s41929-018-0195-1.
- [49] A. Akhoondi, A. Sharma, D. Pathak, M. Yusuf, T.B. Demissie, et al., Hydrogen evolution via noble metals based photocatalysts: A review. Synth. Sinter. 1 (2021) 223–241. https://doi.org/10.53063/synsint.2021.1468.
- [50] L. Tian, Z. Li, M. Song, J. Li, Recent progress in water-splitting electrocatalysis mediated by 2D noble metal materials, Nanoscale. 13 (2021) 12088–12101. https://doi.org/10.1039/D1NR02232F.
- [51] M. Mirzaei, A. Akhoondi, W. Hamd, J.N. Díaz de León, R. Selvaraj, New updates on vanadate compounds synthesis and visible-lightdriven photocatalytic applications, Synth. Sinter. 3 (2023) 28–45. https://doi.org/10.53063/synsint.2023.31132.
- [52] N. Li, Z. Zeng, Y. Zhang, X. Chen, Z. Kong, et al., Double Transition Metal Carbides MXenes (D-MXenes) as Promising Electrocatalysts for Hydrogen Reduction Reaction: Ab Initio Calculations, ACS Omega. 6 (2021) 23676–23682. https://doi.org/10.1021/acsomega.1c00870.

- [53] Z. Zeng, X. Chen, K. Weng, Y. Wu, P. Zhang, et al., Computational screening study of double transition metal carbonitrides M'2M"CNO2-MXene as catalysts for hydrogen evolution reaction, npj Comput. Mater. 7 (2021) 80. https://doi.org/10.1038/s41524-021-00550-4.
- [54] A. Kahn, Fermi level, work function and vacuum level, Mater Horiz. 3 (2016) 7–10. https://doi.org/10.1039/C5MH00160A.
- [55] W. Sun, Y. Xie, P. Kent, Double transition metal MXenes with wide band gaps and novel magnetic properties, Nanoscale. 10 (2018) 11962–11968. https://doi.org/10.1039/C8NR00513C.
- [56] R. Jayan, A. Vashisth, M.M. Islam, First-principles investigation of elastic and electronic properties of double transition metal carbide MXenes, J. Am. Ceram. Soc. 105 (2022) 4400–4413. https://doi.org/10.1111/jace.18394.
- [57] D. Jin, P. Hou, Y. Tian, X. Liu, Y. Xie, et al., Single transition metal atom stabilized on double metal carbide MXenes for hydrogen evolution reaction: a density functional theory study, J. Phys. D: Appl. Phys. 55 (2022) 444002. https://doi.org/10.1088/1361-6463/ac8a5a.
- [58] L.-H. Zheng, C.-K. Tang, Q.-F. Lü, J. Wu, MoS2/Mo2TiC2Tx supported Pd nanoparticles as an efficient electrocatalyst for hydrogen evolution reaction in both acidic and alkaline media, Int. J. Hydrog. Energy. 47 (2022) 11739–11749. https://doi.org/10.1016/j.ijhydene.2022.01.201.
- [59] J. Li, C. Chen, Z. Lv, W. Ma, M. Wang, et al., Constructing heterostructures of ZIF-67 derived C, N doped Co2P and Ti2VC2Tx MXene for enhanced OER, J. Mater. Sci. Technol. 145 (2023) 74–82. https://doi.org/10.1016/j.jmst.2022.10.048.
- [60] D. Jin, L.R. Johnson, A.S. Raman, X. Ming, Y. Gao, et al., Computational Screening of 2D Ordered Double Transition-Metal Carbides (MXenes) as Electrocatalysts for Hydrogen Evolution Reaction, J. Phys. Chem. C. 124 (2020) 10584–10592. https://doi.org/10.1021/acs.jpcc.0c01460.
- [61] O. Mashtalir, M. Naguib, V.N. Mochalin, Y. Dall'Agnese, M. Heon, et al., Intercalation and delamination of layered carbides and carbonitrides, Nat. Commun. 4 (2013) 1716. https://doi.org/10.1038/ncomms2664.
- [62] X. Song, H. Wang, S. Jin, M. Lv, Y. Zhang, et al., Oligolayered Ti3C2Tx MXene towards high performance lithium/sodium storage, Nano Res. 13 (2020) 1659–1667. https://doi.org/10.1007/s12274-020-2789-6.
- [63] K. Kannan, K.K. Sadasivuni, A.M. Abdullah, B. Kumar, Current Trends in MXene-Based Nanomaterials for Energy Storage and Conversion System: A Mini Review, Catalysts. 10 (2020) 495. https://doi.org/10.3390/catal10050495.
- [64] M. Zhou, Y. Shen, J.J. Liu, L.L. Lv, Y. Zhang, et al., Excellent double metal MXenes MoWC anode: The synergistic effect of molybdenum and tungsten transition metal, Vacuum. 213 (2023) 112152. https://doi.org/10.1016/j.vacuum.2023.112152.
- [65] A. Samad, A. Shafique, H.J. Kim, Y.-H. Shin, Superionic and electronic conductivity in monolayer W2C: ab initio predictions, J. Mater. Chem. A. 5 (2017) 11094–11099. https://doi.org/10.1039/C7TA01177F.
- [66] V. Mehta, H.S. Saini, S. Srivastava, M.K. Kashyap, K. Tankeshwar, Ultralow diffusion barrier of double transition metal MoWC monolayer as Li-ion battery anode, J. Mater. Sci. 57 (2022) 10702– 10713. https://doi.org/10.1007/s10853-022-07237-1.
- [67] Q. Sun, Y. Dai, Y. Ma, T. Jing, W. Wei, B. Huang, Ab Initio Prediction and Characterization of Mo2C Monolayer as Anodes for Lithium-Ion and Sodium-Ion Batteries, J. Phys. Chem. Lett. 7 (2016) 937–943. https://doi.org/10.1021/acs.jpclett.6b00171.
- [68] M. Zhou, Y. Shen, J.J. Liu, L.L. Lv, X. Gao, et al., Superionic conductivity and large capacitance behaviors of two-metal MXenes WCrC in sodium ion battery, Vacuum. 200 (2022) 111054. https://doi.org/10.1016/j.vacuum.2022.111054.
- [69] Y.-M. Li, W.-G. Chen, Y.-L. Guo, Z.-Y. Jiao, Theoretical investigations of TiNbC MXenes as anode materials for Li-ion

batteries, J. Alloys Compd. 778 (2019) 53–60. https://doi.org/10.1016/j.jallcom.2018.11.140.

- [70] S. Zhao, W. Kang, J. Xue, Role of Strain and Concentration on the Li Adsorption and Diffusion Properties on Ti2C Layer, J. Phys. Chem. C. 118 (2014) 14983–14990. https://doi.org/10.1021/jp504493a.
- [71] J. Hu, B. Xu, C. Ouyang, Y. Zhang, S.A. Yang, Investigations on Nb2C monolayer as promising anode material for Li or non-Li ion batteries from first-principles calculations, RSC Adv. 6 (2016) 27467–27474. https://doi.org/10.1039/C5RA25028E.
- [72] X. Li, Y. Pang, M. Wang, X. Zhang, Z. Lu, Z. Yang, The synergistic effect of Ti and Nb in TiNbC leads to enhanced anode performance for Na-ion batteries - first-principles calculations, Phys. Scr. 98 (2023) 025710. https://doi.org/10.1088/1402-4896/acb46a.
- [73] W. Liu, J. Cao, F. Song, D.-D. Zhang, M. Okhawilai, et al., A double transition metal Ti2NbC2Tx MXene for enhanced lithium-ion storage, Rare. Met. 42 (2023) 100–110. https://doi.org/10.1007/s12598-022-02120-z.
- [74] X. Guo, X. Xie, S.J. Choi, Y. Zhao, H. Líu, et al., Sb2O3/MXene(Ti3C2Tx) hybrid anode materials with enhanced performance for sodium-ion batteries Sb2O3/MXene(Ti3C2Tx) hybrid anode materials with enhanced performance for sodium-ion batteries, J. Mater. Chem. A. 5 (2017) 12445–12452. https://doi.org/10.1039/C7TA02689G.
- [75] Z. Dai, J. Cao, F. Song, D. Zhang, J. Qin, X. Zhang, Architecting Nb-TiO2-x/(Ti0.9Nb0.1)3C2Tx MXene Nanohybrid Anode for High-Performance Lithium-Ion Batteries, Adv. Mater. Interfaces. 9 (2022) 2101658. https://doi.org/10.1002/admi.202101658.
- [76] C. Xu, K. Feng, X. Yang, Y. Cheng, X. Zhao, et al., In-situ construction of metallic oxide (VNbO5) on VNbCTx MXene for enhanced Li-ion batteries performance, J. Energy Storage. 69 (2023) 107888. https://doi.org/10.1016/j.est.2023.107888.
- [77] Y. Cheng, L. Yang, S. Yin, Synthesis and lithium ion storage performance of novel two dimensional vanadium niobium carbide (VNbCTx) MXene, Compos. Commun. 40 (2023) 101588. https://doi.org/10.1016/j.coco.2023.101588.
- [78] Y. Li, L. Li, R. Huang, Y. Zhang, Y. Wen, Computational screening of pristine and functionalized ordered TiVC MXenes as highly efficient anode materials for lithium-ion batteries, Nanoscale. 13 (2021) 2995–3001. https://doi.org/10.1039/D0NR08271F.
- [79] S.-P. Huang, J. Zhang, Y.-R. Ren, W.-K. Chen, Investigating the potentials of TiVC MXenes as anode materials for Li-ion batteries by DFT calculations, Appl. Surf. Sci. 569 (2021) 151002. https://doi.org/10.1016/j.apsusc.2021.151002.
- [80] K. Feng, Y. Li, C. Xu, M. Zhang, X. Yang, et al., In-situ partial oxidation of TiVCTx derived TiO2 and V2O5 nanocrystals functionalized TiVCTx MXene as anode for lithium-ion batteries, Electrochim. Acta. 444 (2023) 142022. https://doi.org/10.1016/j.electacta.2023.142022.
- [81] Y. Li, J. Zhang, Y. Cheng, K. Feng, J. Li, et al., Stable TiVCTx/poly-o-phenylenediamine composites with threedimensional tremella-like architecture for supercapacitor and Li-ion battery applications, Chem. Eng. J. 433 (2022) 134578. https://doi.org/10.1016/j.cej.2022.134578.
- [82] Y. Cheng, Y. Li, L. Yang, S. Yin, Poly(o-phenylenediamine)-Decorated V4C3Tx MXene/Poly(o-phenylenediamine) Blends as Electrode Materials to Boost Storage Capacity for Supercapacitors and Lithium-Ion Batteries, ACS Appl. Nano Mater. 6 (2023) 9186– 9196. https://doi.org/10.1021/acsanm.3c00624.
- [83] K. Chen, Y. Guan, L. Tan, H. Zhu, Q. Zhang, et al., Atomically selective oxidation of (Ti,V) MXene to construct TiO2@TiVCTx heterojunction for high-performance Li-ion batteries, Appl. Surf. Sci. 617 (2023) 156575. https://doi.org/10.1016/j.apsusc.2023.156575.
- [84] T.L. Tan, H.M. Jin, M.B. Sullivan, B. Anasori, Y. Gogotsi, High-Throughput Survey of Ordering Configurations in MXene Alloys Across Compositions and Temperatures, ACS Nano. 23 (2017) 4407–4418. https://doi.org/10.1021/acsnano.6b08227.

- [85] S.-P. Huang, J.-F. Gu, Y.-R. Ren, K.-N. Ding, Y. Li, et al., Investigation of Ordered TiMC and TiMCT2 (M = Cr and Mo; T = O and S) MXenes as High-Performance Anode Materials for Lithium-Ion Batteries, J. Phys. Chem. C. 126 (2022) 5283–5291. https://doi.org/10.1021/acs.jpcc.1c10638.
- [86] H. Wang, Z. Jing, H. Liu, X. Feng, G. Meng, et al., A highthroughput assessment of the adsorption capacity and Li-ion diffusion dynamics in Mo-based ordered double-transition-metal MXenes as anode materials for fast-charging LIBs, Nanoscale. 12 (2020) 24510–24526. https://doi.org/10.1039/D0NR05828A.
- [87] M. Zhou, Y. Shen, J.J. Liu, L.L. Lv, Y. Zhang, et al., Collaborative activation mechanism in double transition metal MXenes anode: An effective method to improve the capacitance of sodium ion battery, Vacuum. 213 (2023) 112150. https://doi.org/10.1016/j.vacuum.2023.112150.
- [88] J. Hu, B. Xu, C. Ouyang, S.A. Yang, Y. Yao, Investigations on V2C and V2CX2 (X = F, OH) Monolayer as a Promising Anode Material for Li Ion Batteries from First-Principles Calculations, J. Phys. Chem. C. 118 (2014) 24274–24281. https://doi.org/10.1021/jp507336x.
- [89] V. Mehta, H.S. Saini, S. Srivastava, M.K. Kashyap, K. Tankeshwar, N-based single and double transition metal V2N/CrVN monolayers as high capacity anode materials for Li-ion batteries, Mater. Chem. Phys. 290 (2022) 126531. https://doi.org/10.1016/j.matchemphys.2022.126531.
- [90] R. Syamsai, J.R. Rodriguez, V.G. Pol, Q.V. Le, K.M. Batoo, et al., Double transition metal MXene (TixTa4-xC3) 2D materials as anodes for Li-ion batteries, Sci. Rep. 11 (2021) 688. https://doi.org/10.1038/s41598-020-79991-8.
- [91] M. Naguib, J. Come, B. Dyatkin, V. Presser, P.-L. Taberna, et al., MXene: a promising transition metal carbide anode for lithium-ion batteries, Electrochem. Commun. 16 (2021) 61–64. https://doi.org/10.1016/j.elecom.2012.01.002.
- [92] Y.-C. Lin, R. Torsi, R. Younas, C.L. Hinkle, A.F. Rigosi, et al., Recent Advances in 2D Material Theory, Synthesis, Properties, and Applications, ACS Nano. 17 (2023) 9694–9747. https://doi.org/10.1021/acsnano.2c12759.
- [93] J.P. Singh, R. Bhardwaj, A. Sharma, B. Kaur, S.O. Won, et al., Fabrication of Magnetic Tunnel Junctions, Advanced Applications in Manufacturing Enginering, Woodhead Publishing. (2019) 53–77. https://doi.org/10.1016/B978-0-08-102414-0.00002-1.
- [94] S. Peng, Y. Zhang, M.X. Wang, Y.G. Zhang, W. Zhao, Magnetic Tunnel Junctions for Spintronics: Principles and Applications, Wiley Encyclopedia of Electrical and Electronics Engineering, John Wiley & Sons, Ltd. (2014). https://doi.org/10.1002/047134608X.W8231.
- [95] Z. Cui, Y. Zhang, R. Xiong, C. Wen, J. Zhou, et al., Giant tunneling magnetoresistance in two-dimensional magnetic tunnel junctions based on double transition metal MXene ScCr2C2F2, Nanoscale Adv. 4 (2022) 5144–5153. https://doi.org/10.1039/D2NA00623E.
- [96] J. Neugebauer, T. Hickel, Density functional theory in materials science, WIREs Comput. Mol. Sci. 3 (2013) 438–448. https://doi.org/10.1002/wcms.1125.
- [97] L. Dong, H. Kumar, B. Anasori, Y. Gogotsi, V.B. Shenoy, Rational Design of Two-Dimensional Metallic and Semiconducting Spintronic Materials Based on Ordered Double-Transition-Metal MXenes, J. Phys. Chem. Lett. 8 (2017) 422–428. https://doi.org/10.1021/acs.jpclett.6b02751.
- [98] K. Hantanasirisakul, B. Anasori, S. Nemsak, J.L. Hart, J. Wu, et al., Evidence of a magnetic transition in atomically thin Cr2TiC2Tx MXene, Nanoscale Horiz. 5 (2020) 1557–1565. https://doi.org/10.1039/D0NH00343C.
- [99] I. Borge-Durán, A. Paul, I. Grinberg, From Non-Magnetic to Magnetic: A First-Principles Study of the Emergence of Magnetism in 2D (Nb1-xTix)4C3 MXenes, Chem. Mater. 35 (2023) 7442–7449. https://doi.org/10.1021/acs.chemmater.3c00367.
- [100] Q. Wang, L. Cao, S.-J. Liang, W. Wu, G. Wang, et al., Efficient Ohmic contacts and built-in atomic sublayer protection in MoSi2N4

and WSi2N4 monolayers, npj 2D Mater. Appl. 5 (2021) 71. https://doi.org/10.1038/s41699-021-00251-y.

- [101] Q. Wu, L. Cao, Y.S. Ang, L.K. Ang, Semiconductor-to-metal transition in bilayer MoSi2N4 and WSi2N4 with strain and electric field Scilightfeatured, Appl. Phys. Lett. 118 (2021) 113102. https://doi.org/10.1063/5.0044431.
- [102] A. Kelly, Composites in context, Compos. Sci. Technol. 23 (1985) 171–199. https://doi.org/10.1016/0266-3538(85)90017-X.
- [103] H. Huang, R. Jiang, Y. Feng, H. Ouyang, N. Zhou, et al., Recent development and prospects of surface modification and biomedical applications of MXenes, Nanoscale. 12 (2020) 1325–1338. https://doi.org/10.1039/C9NR07616F.
- [104] J. Xi, X. Liu, L. Zhang, Z. Zhang, J. Zhuo, et al., Engineering of Schottky heterojunction in Ru@Bi2S3/Nb2C MXene based on work function with enhanced carrier separation for promoted sterilization, Chem. Eng. J. 473 (2023) 145169. https://doi.org/10.1016/j.cej.2023.145169.
- [105] H. Frei, Photocatalytic fuel production, Curr. Opin. Electrochem. 2 (2017) 128–135. https://doi.org/10.1016/j.coelec.2017.03.009.
- [106] Z. Qin, T. Su, H. Ji, MXene-Based Photocatalysts Fabrication and Applications, CRC Press., Boca Raton. (2022). https://doi.org/10.1201/9781003156963.
- P.M. Patterson, T.K. Das, B.H. Davis, Carbon monoxide hydrogenation over molybdenum and tungsten carbides, Appl. Catal.
 A. 251 (2003) 449–455. https://doi.org/10.1016/S0926-860X(03)00371-5.
- [108] A.B. Vidal, L. Feria, J. Evans, Y. Takahashi, P. Liu, et al., CO2 Activation and Methanol Synthesis on Novel Au/TiC and Cu/TiC Catalysts, J. Phys. Chem. Lett. 3 (2013) 2275–2280. https://doi.org/10.1021/jz300989e.
- [109] Y. Cheng, X. Xu, Y. Li, Y. Zhang, Y. Song, CO2 reduction mechanism on the Nb2CO2 MXene surface: Effect of nonmetal and metal modification, Comput. Mater. Sci. 202 (2022) 110971. https://doi.org/10.1016/j.commatsci.2021.110971.
- [110] H. Zhou, Z. Chen, E. Kountoupi, A. Tsoukalou, P.M. Abdala, et al., Two-dimensional molybdenum carbide 2D-Mo2C as a superior catalyst for CO2 hydrogenation, Nat. Commun. 12 (2021) 5510. https://doi.org/10.1038/s41467-021-25784-0.
- [111] Z. Wu, J. Shen, C. Li, C. Zhang, K. Feng, et al., Mo2TiC2 MXene-Supported Ru Clusters for Efficient Photothermal Reverse Water–Gas Shift, ACS Nano. 17 (2023) 1550–1559. https://doi.org/10.1021/acsnano.2c10707.
- [112] N. Mwankemwa, H.-E. Wang, T. Zhu, Q. Fan, F. Zhang, et al., First principles calculations investigation of optoelectronic properties and photocatalytic CO2 reduction of (MoSi2N4)5-n/(MoSiGeN4)n in-plane heterostructures, Results Phys. 37 (2022) 105549. https://doi.org/10.1016/j.rinp.2022.105549.
- [113] F. Wöhler, Ueber künstliche Bildung des Harnstoffs, Ann. Phys. Chem. 88 (1828) 253–256. https://doi.org/10.1002/andp.18280880206.
- [114] Y. Yang, J. Peng, Z. Shi, P. Zhang, A. Arramel, N. Li, Unveiling the key intermediates in electrocatalytic synthesis of urea with CO2 and N2 coupling reactions on double transition-metal MXenes, J. Mater. Chem. A. 11 (2023) 6428–6439. https://doi.org/10.1039/D2TA09477K.
- [115] S. Zhang, J. Geng, Z. Zhao, M. Jin, W. Li, et al., Highefficiency electrosynthesis of urea over bacterial cellulose regulated Pd–Cu bimetallic catalyst, EES. Catal. 1 (2023) 45–53. https://doi.org/10.1039/D2EY00038E.

- [116] Z. Li, N.H. Attanayake, J.L. Blackburn, E.M. Miller, Carbon dioxide and nitrogen reduction reactions using 2D transition metal dichalcogenide (TMDC) and carbide/nitride (MXene) catalysts, Energy Environ. Sci. 14 (2021) 6242–6286. https://doi.org/10.1039/D1EE03211A.
- [117] L. Li, X. Wang, H. Guo, G. Yao, H. Yu, et al., Theoretical Screening of Single Transition Metal Atoms Embedded in MXene Defects as Superior Electrocatalyst of Nitrogen Reduction Reaction, Small Methods. 3 (2019) 1900337. https://doi.org/10.1002/smtd.201900337.
- [118] R. Zhao, Y. Chen, H. Xiang, Y. Guan, C. Yang, et al., Two-Dimensional Ordered Double-Transition Metal Carbides for the Electrochemical Nitrogen Reduction Reaction, ACS Appl. Mater. Interfaces. 15 (2023) 6797–6806. https://doi.org/10.1021/acsami.2c19911.
- [119] Q.-J. Fang, W. Zhang, Q.-j. Zhang, J.-h. Wang, S.-t. Zhao, et al., Rational design of bimetallic MXene solid solution with High-Performance electrocatalytic N2 reduction, J. Colloid Interface Sci. 640 (2023) 67–77. https://doi.org/10.1016/j.jcis.2023.02.094.
- [120] R. Khan, S. Andreescu, MXenes-Based Bioanalytical Sensors: Design, Characterization, and Applications, Sensors. 20 (2020) 5434. https://doi.org/10.3390/s20185434.
- [121] S. Alwarappan, N. Nesakumar, D. Sun, T. Y. Hu, C.-Z. Li, 2D metal carbides and nitrides (MXenes) for sensors and biosensors, Biosens. Bioelectron. 205 (2022) 113943. https://doi.org/10.1016/j.bios.2021.113943.
- [122] A. Bafekry, M. Faraji, M.M. Fadlallah, A. Abdolahzadeh Ziabari, A. Bagheri Khatibani, et al., Adsorption of habitat and industry-relevant molecules on the MoSi2N4 monolayer, Appl. Surf. Sci. 564 (2021) 150326. https://doi.org/10.1016/j.apsusc.2021.150326.
- [123] H. Vovusha, R.G. Amorim, H. Bae, S. Lee, T. Hussain, H. Lee, Sensing of sulfur containing toxic gases with double transition metal carbide MXenes, Mater. Today Chem. 30 (2023) 101543. https://doi.org/10.1016/j.mtchem.2023.101543.
- [124]. J. Xu, Y. Sun, J. Zeng, F. Zhang, W. Zhang, The electronic and optical properties, gas sensor and NO removal application investigations of noble metal-adsorbed MoSi2N4, Results Phys. 49 (2023) 106481. https://doi.org/10.1016/j.rinp.2023.106481.
- [125] Y. Linghu, T. Tong, C. Wu, Cu-Doped MoSi2N4 Monolayer as a Potential NH3 Sensor, ChemPhysChem. 24 (2023) e202200712. https://doi.org/10.1002/cphc.202200712.
- [126] M. Li, Z. Li, P. Wang, Q. Ma, A novel bimetallic MXene derivative QD-based ECL sensor for miRNA-27a-3p detection, Biosens. Bioelectron. 228 (2023) 115225. https://doi.org/10.1016/j.bios.2023.115225.
- [127] G. Li, B. Zhou, P. Wang, M. He, Z. Fang, et al., High-Efficiency Oxygen Reduction to Hydrogen Peroxide Catalyzed by Oxidized Mo2TiC2 MXene, Catalysts. 12 (2022) 850. https://doi.org/10.3390/catal12080850.
- [128] Y. Gao, L. Pan, Q. Wu, X. Zhuang, G. Tan, Q. Man, Honeycomb-like SnS2/graphene oxide composites for enhanced microwave absorption, J. Alloys Compd. 915 (2022) 165405. https://doi.org/10.1016/j.jallcom.2022.165405.
- [129] Y. Bao, Y. Liu, Z. Zhang, J. Pan, X. Li, et al., Constructing 2D/2D ultrathin Ti3C2/SnS2 Schottky heterojunctions toward efficient tetracycline degradation, Chemosphere. 307 (2022) 136118. https://doi.org/10.1016/j.chemosphere.2022.136118.