Electronic and Optical Properties of 2D Transition Metal Carbides and Nitrides (MXenes)

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2D transition metal carbides, carbonitrides, and nitrides, known as MXenes, are a rapidly growing family of 2D materials with close to 30 members experimentally synthesized, and dozens more studied theoretically. They exhibit outstanding electronic, optical, mechanical, and thermal properties with versatile transition metal and surface chemistries. They have shown promise in many applications, such as energy storage, electromagnetic interference shielding, transparent electrodes, sensors, catalysis, photothermal therapy, etc. The high electronic conductivity and wide range of optical absorption properties of MXenes are the key to their success in the aforementioned applications. However, relatively little is currently known about their fundamental electronic and optical properties, limiting their use to their full potential. Here, MXenes’ electronic and optical properties from both theoretical and experimental perspectives, as well as applications related to those properties, are discussed, providing a guide for researchers who are exploring those properties of MXenes.

1. Introduction

2D materials became the focus of material research in the past decade owing to their unique electronic, optical, mechanical, and thermal properties that are different from their bulk counterparts.[1] For examples, charge carriers in graphene can be described as massless Dirac fermions with extremely high mobility exceeding 10 000 V cm−1 s−1.[2] Transition metal dichalcogenides transform from indirect to direct bandgap semiconductors with spin-valley coupling in the monolayer state.[1,4] Titanium oxide nanosheets exhibit large dielectric constant and electronic permittivity that are suitable for modern electronic devices.[3] These unique properties are the result of quantum confinement effect in the atomically thin 2D layers and are strongly dependent on the layer thickness and composition. Moreover, the properties of 2D materials are highly tunable by chemical doping, strain engineering, and external fields which enable precise control of their properties.[6–9]

The discovery of 2D titanium carbide (Ti3C2) in 2011 added a new family of materials known as MXenes to the 2D world.[10] In general, the term MXenes refers to a large family of 2D transition metal carbides, carbonitrides, and nitrides with the formula M_{n+1}X_nTx, where M represents an early transition metal, X is carbon and/or nitrogen, and T_x stands for surface terminations (such as OH, O, and F). Typically, MXenes are produced by selective etching of A elements from MAX phases, where A is a group IIIA to VIA element (Figure 1), but other precursors and methods of synthesis are also being explored.[11] MXenes exhibit a unique combination of metallic conductivity due to free electrons of transition metal carbide or nitride backbone and hydrophilicity resulting from their surface terminations. Because of their high electronic conductivity and versatile chemistry, they have shown promise in a variety of applications including energy storage,[12] electromagnetic interference (EMI) shielding,[12] transparent conductors,[13,14] gas and pressure sensors,[15–18] water purification,[19–22] photo- and electrocatalysis,[23,24] thermoelectrics,[25,26] and plasmonics.[27,28] Due to a large variety of transition metals and surface functionalities, MXenes’ properties can be tuned by selecting combinations of transition metals, X elements, and controlling their surface chemistries. Close to 30 MXenes have been experimentally reported (marked with green color in Figure 1), whereas many more are predicted to exist and have been studied theoretically (marked with black color in Figure 1).[29–45] Given that close to 100 MAX phases have been made, not counting unlimited solid solutions and a number of ordered double transition metal structures,[46,47] there are endless and quickly expanding opportunities for producing MXenes with desirable properties.

It is clear from a large number of MXene-related publications that this family of materials attracts great attention from various research communities including material scientists, chemists, and physicists, due to their promising properties in many applications and fascinating chemistry and physics resulting from their 2D nature. Comprehensive reviews on MXenes synthesis, energy storage and conversion, catalysis, sensors, electronic, and biomedical applications were recently published.[11,35,48–56] Many interesting electronic properties of MXenes such as being topological insulator (quantum spin Hall effect), metal-to-insulator transition, and superconductivity have been predicted but still await experimental confirmation.[57–61] Moreover, their fundamental properties such as the intrinsic electronic transport, interaction of MXene flakes with electromagnetic waves, and mechanical behavior of a single...
MXene flake is still poorly understood. Mechanical properties of $\text{Ti}_3\text{C}_2\text{T}_x$ mono- and bilayers were reported only recently. This review focuses largely on electronic and optical properties of MXenes aiming not only to summarize studies of those properties, but also to bridge the gap between theoretical predictions and experiments. We begin with a brief overview of synthesis and processing of MXenes to the extent that they affect the structure and surface chemistry. Then we provide highlights of theoretical studies, describe experimental measurements of electronic and transport properties, and effects of surface modification on electronic properties. Then we discuss some applications that are related to superior electronic conductivity of MXenes such as EMI shielding, pressure and molecular sensors, and transparent conductors. After that, we move on to optical properties of MXenes and their applications in ultrafast lasers, plasmonics, and photothermal therapy. In each section, we also discuss experiments that could be performed to further explore the electronic and optical properties of MXenes. Finally, we conclude this review with a description of the challenges and an outlook for future research in this field. We hope that this review will be a useful guide to both theorists and experimentalists who are exploring electronic and optical properties of this relatively new, but quickly expanding family of materials.

2. Synthesis and Processing

MXenes are produced mainly by selective etching of A elements from their parent MAX phases as shown for $\text{Ti}_3\text{C}_2\text{T}_x$ MXene in Figure 2. This process is possible because of high selectivity of HF-based etchant that allowed even selective etching of SiC polypolytypes. Metallic M–A bonds are more reactive than mixed metallic/ionic/covalent M–X bonds in a fluoride-containing etchant. MXenes were first produced only by etching in HF aqueous solution with different concentrations and conditions depending on the MAX phases. Later, a mixture of LiF and HCl solution was shown to successfully produce $\text{Ti}_3\text{C}_2\text{T}_x$, $\text{Ti}_3(\text{C,N})_2\text{T}_x$, and $\text{Ti}_2\text{CT}_x$. There have also been reports of hydrothermal etching of MAX phases to produce MXenes. Moreover, $\text{Ti}_3\text{C}_2\text{T}_x$ can also be produced from biafluoride salt ($\text{NH}_4\text{HF}_2$). A detailed synthesis protocol for producing $\text{Ti}_3\text{C}_2\text{T}_x$ was recently published. Note that synthesis conditions used for one MXene should not be generalized to other MXenes as each MAX phase has its own stability and reactivity toward different etchants. Generally, $M_3\text{AX}_x$ (413 phase) requires more aggressive etching conditions than $M_2\text{AX}_x$ (312 phase) and $M_4\text{AX}$ (211 phase). From more than 10 A elements present in MAX phases (Figure 1), only Al and Si have been successfully etched to produce MXenes so far. Etching Si from $\text{Ti}_3\text{SiC}_2$ or $\text{Ti}_3\text{C}_2\text{T}_x$ MXene was reported only recently and required a use of oxidant, like in the case of etching SiC. Another thing to keep in mind regarding etching process is that aggressive etching conditions (high HF concentration, high temperature, long etching time, use of Cl$_2$ etchant) can cause over-etching, resulting in defects in the M sites or complete removal of both A and M elements yielding carbide-derived carbon. It follows that a balance between etching and MAX stability must be established to obtain 2D MXenes with desired properties.

During the chemical etching process, Al layers in MAX phases react with HF (or fluoride ions) to form $\text{AlF}_3$ and gaseous hydrogen, causing MXene layers to exfoliate according to Equation (1). Moreover, the surface transition metal spontaneously reacts with water or fluoride ions forming OH, O, and/or F surface terminations (Equations (2) and (3)).

$$M_{\text{al}}\text{AlX}_3(\nu)+3\text{HF}(\nu) \rightarrow M_{\text{al}}\text{X}_3(\nu)+\text{AlF}_3(\nu)+3/2\text{H}_2(\nu) \quad (1)$$

$$M_{\text{al}}\text{X}_3(\nu)+2\text{H}_2\text{O}(\nu) \rightarrow M_{\text{al}}\text{X}_3(\nu)+\text{OH}_2(\nu)+\text{H}_2(\nu) \quad (2)$$

$$M_{\text{al}}\text{X}_3(\nu)+2\text{HF}(\nu) \rightarrow M_{\text{al}}\text{X}_3(\nu)+\text{H}_2(\nu) \quad (3)$$

MXenes produced from chemical etching are always terminated by O, OH, F or more likely, a combination of all species. The amount of each termination depends on the nature of the transition metal on MXene surface, e.g., Mo is less favorable to bond with F compared to Ti. Another thing to keep in mind regarding etching process is that aggressive etching conditions (high HF concentration, high temperature, long etching time, use of Cl$_2$ etchant) can cause over-etching, resulting in defects in the M sites or complete removal of both A and M elements yielding carbide-derived carbon. It follows that a balance between etching and MAX stability must be established to obtain 2D MXenes with desired properties.

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complexity of surface terminations. Moreover, producing uniform terminations and nonterminated MXenes remains challenging, as will be discussed in the next section of this review.

It was shown that HF can also be used to etch non-MAX phases to produce MXenes. For examples, etching of two Ga layers from Mo$_2$Ga$_2$C to produce Mo$_2$CT$_x$ MXene was reported.[31,89] Moreover, Zhou et al. reported etching of Al$_3$C$_2$ layers from Zr$_3$Al$_3$C$_5$ to produce Zr$_3$C$_2$T$_x$, the first and only Zr-based MXene reported to date.[39] Recently, the same group also reported successful preparation of Hf$_3$C$_2$T$_x$ by substitution of Si on Al site in Hf$_3$Al$_4$C$_6$ followed by etching of [Al(Si)$_4$]$_4$C$_4$ layer.[40] These results show that it is possible to produce MXenes even when MAX phase precursors are not available, providing more options for MXenes synthesis.

While several carbide and carbonitride MXenes were successfully synthesized by wet chemical etching, this method was able to produce only Ti$_2$NT$_x$ nitride MXene so far.[43] This is possibly due to high formation energy and low cohesive energy of nitride MXenes compared to the carbide counterparts.[90] Etching Ti$_4$AlN$_3$ in HF solution results in dissolution of Ti$_4$AlN$_3$ instead of Ti$_4$N$_3$T$_x$ MXene formation.[91] Instead, Ti$_4$NT$_x$ MXene was prepared by treating Ti$_4$AlN$_3$ in a molten fluoride salt at 550 °C.[33] More recently, Mo$_2$NT$_x$ and V$_2$NT$_x$ were synthesized by ammoniation of Mo$_2$CT$_x$ and V$_2$CT$_x$ MXenes with NH$_3$ gas at 550 °C.[30] This method results in transformation of Mo- and V-based carbide MXenes to nitride MXenes. However, cubic VN was also formed in addition to V$_2$NT$_x$ MXene.

Delamination step is necessary to obtain mono- or few-layer MXene flakes (step 2 in Figure 2). Since the strong M–A bonds are replaced by weaker van der Waals and hydrogen bonds during etching, multilayered MXenes can readily be delaminated. However, the interlayer interaction in MXenes is still 2–6 times stronger than that of graphite.[92] Therefore, mechanical exfoliation by Scotch tape method did not result in a MXene monolayer.[86,93] Generally, delamination of MXenes is achieved by intercalation followed by mechanical agitation. For HF-etched MXenes, organic intercalants such as dimethyl sulfoxide (DMSO), tetraalkylammonium hydroxide, isopropylamine, hydrazine, or urea are used to expand MXene interlayer distance.[94,95] For MXenes etched by a mixture of LiF and HCl, Li$^+$ cations readily intercalate MXene layers causing them to expand without the need for additional intercalant.[63,72] Depending on desired flake size, flake quality, and concentration of MXene solution, hand-shaking, bath sonication, or probe sonication of...
the intercalated ML-MXenes are used to separate MXene layers. While hand-shaking generally results in larger MXene flakes (5–15 µm) and fewer defects, sonication leads to a high concentration colloidal solution of delaminated (d-) MXene. Delamination techniques that could produce MXene monolayer with large lateral size still need further development. The d-MXene colloidal solution containing mono- or few-layer MXene flakes is stable against aggregation due to its high negative zeta potential.[96] This solution can be processed in different ways, such as vacuum filtration to form free-standing MXene “paper,” spin or spray coating,[13,14] painting,[97] printing, stamping,[98] electrophoresis,[99] or forming polymer composites and fibers (step 3 in Figure 2).[100] Moreover, Ti3C2Tx MXene can be re-dispersed in a wide variety of polar organic solvents suitable for further processing.[101] MXene flakes are fairly easily oxidized in ambient atmosphere, especially in O2-containing aqueous solution.[102,103] Therefore, it is recommended that MXene solutions are used soon after preparation, or stored refrigerated in deaerated water or organic solvent.

For electronic and optical studies, large lateral-size and high-quality MXene flakes are preferable. MXene flakes resulting from wet chemical etching are usually less than 10 µm in lateral-size, and likely contain atomic defects.[94] Chemical vapor deposition (CVD) has been used to prepare several micrometer-wide Mo2C crystal, it was possible that the Mo2C crystals produced by this method were orthorhombic (α-Mo2C) similar to previous report due to high growth temperature.[104] A more recent work on carburization of MoS2 was reported to produce atomically sharp lateral heterojunction between Mo2C and MoS2.[106] High-resolution transmission electron microscopy (HRTEM) and electron diffraction showed that the Mo2C crystal growth by this method had different crystal structure from the hexagonal MoS2 precursor, suggesting that Mo2C crystal resulting from this method is different from the hexagonal structure of Mo2C MXene. Recently, homoepitaxial growth of hexagonal TiC single layers on a Ti3C2Tx flake was achieved by combined thermal annealing and electron-beam irradiation inside a transmission electron microscopy (TEM).[107] To progressively study intrinsic electronic and optical properties of MXenes, it is crucial to develop CVD or other bottom-up synthesis methods that produce high-quality monolayer MXenes with large lateral size and controllable or no surface termination.[108]

3. Structure and Surface Chemistry

MXenes inherit hexagonal symmetry with P6_3/mmc space group from their parent MAX precursors, where the transition metal (M) atoms are arranged in a nearly close-packed structure.
with X element atoms in the octahedral interstitial sites, as shown in Figure 3a,b. In the Al-containing MAX phases, the in-plane M–X bond has a mixed covalent/metallic/ionic character, whereas the M–Al bond is metallic, making it possible to selectively etch the Al layer from the MAX phases converting them to MXenes, as discussed in the previous section. After etching, the A layers are replaced by O, OH, and/or F surface terminations bonded to the outer transition metal layers. Moreover, recent study has shown that Cl atoms can also functionalize Ti$_2$CT$_x$ and Ti$_3$C$_2$Tx surface when they are etched in Cl-containing environment. MXenes are likely to stay fully terminated as evidenced from large negative formation energy indicating strong bonding between the transition metals and the surface terminations. Moreover, all positive phonon frequencies of fully terminated MXenes further confirm local stabilization. There are three possible sites for these terminations on MXenes’ surface, i.e., directly on top of transition metal atoms, hollow site I between three neighboring X atoms under the transition metals, and hollow site II on top of the X atoms (Figure 3a,b). Density functional theory (DFT) calculations have shown that surface terminations located at site I on both sides of MXenes sheets is the most stable configuration for most MXenes due to low steric hindrance. However, site II becomes energetically more favorable for MXenes, when the transition metals cannot provide sufficient electrons to both X and surface terminations. In particular, O-termination requires two electrons to stabilize its adsorption position unlike OH- and F-terminations, which only require one electron from the transition metal surface. Therefore, O-terminations in MXenes with low valency transition metals tend to be either in site II configuration or mixed site I and II.

Experimentally, MXenes’ surface terminations are still poorly understood despite use of different characterization techniques for their analysis and monitoring including, X-ray photoelectron spectroscopy (XPS), nuclear magnetic resonance spectroscopy (NMR), neutron scattering, X-ray atomic pair distribution function (X-ray PDF), scanning transmission electron microscopy (STEM), electron energy loss

![Figure 3.](image-url)

Figure 3. Structure and surface chemistry of Ti$_3$C$_2$T$_x$ MXene: a) Side and b) top views of M$_3$X$_2$(OH)$_x$. c,d) High-resolution X-ray photoelectron (XPS) spectra of the O1s region (c) and the F1s region (d). e) $^1$H nuclear magnetic resonance (NMR) spectra of Ti$_3$C$_2$T$_x$ synthesized by different methods. f) Composition of terminations obtained from NMR study suggesting that high F content is found in HF-etched Ti$_3$C$_2$T$_x$. g) Atomic pair distribution function (PDF) obtained from neutron scattering. h) Atomistic model used in the fitting of the PDF data. The Ti, C, O, F, and H atoms are represented by yellow, black, red, green, and white spheres, respectively. c,d) Reproduced with permission. e,f) Reproduced with permission. c,d) Copyright 2016, Elsevier. c,d) Copyright 2016, the Royal Society of Chemistry. g,h) Copyright 2015, American Chemical Society.
The formula of Ti$_3$C$_2$O$_{0.3}$(OH)$_{0.32}$F$_{1.2}$ for Ti$_3$C$_2$T$_x$ and quantify these species. [114,126] Moreover, it was later shown in situ temperature-programmed XPS that the binding energy of the O-termination also depends on the local environment of the adsorption site. [115] For comparison, Halim et al. reported the formula of Ti$_3$C$_2$O$_{0.12}$F$_{0.8}$O$_{0.54}$ and Ti$_3$C$_2$(OH)$_{1.04}$F$_{0.8}$O$_{0.13}$ for Ti$_3$C$_2$T$_x$ MXene etched with 50% HF. [114] On the contrary, Persson et al. reported that Ti$_3$C$_2$T$_x$ MXene etched with 10% HF contained only O-termination located at different adsorption sites with small variation in binding energies. [115] In the former study, binding energies of 529.9, 531.2, and 532.0 eV were assigned to TiO$_2$, O-, and OH-terminations, respectively. On the other hand, the latter study proposed that these positions can all be assigned to O-termination with O atom bridging two Ti sites and O-termination in the absence and in the presence of neighboring F atoms, respectively. [115] More detailed XPS studies are needed to fully understand the surface chemistry of Ti$_3$C$_2$T$_x$ and other MXenes.

Solid-state NMR spectroscopy with high sensitivity toward $^1$H, $^{19}$F, and $^{13}$C nuclei was used to study Ti$_3$C$_2$T$_x$ and V$_2$CT$_x$ MXenes. [116,117] As an example, the $^1$H spectra of Ti$_3$C$_2$T$_x$ are shown in Figure 3e. Note that NMR cannot directly detect O-containing species, and the amount of O-termination is calculated based on the assumption that the total amount of surface terminations (n$_{OH} + n_F + 2n_O$) is equal to 2. Hope et al. reported the formula of Ti$_3$C$_2$O$_{0.12}$F$_{0.54}$ and Ti$_3$C$_2$(OH)$_{0.08}$F$_{0.25}$O$_{0.88}$ for 50% HF-etched and LiF-etched Ti$_3$C$_2T_x$, respectively. [116] These NMR results are in good agreement with the recent XPS study [115] suggesting that dry Ti$_3$C$_2$T$_x$ surface comprises mainly O- and F-terminations with small amount of OH-terminations (Figure 3f). Another NMR study was performed on V$_2$CT$_x$ MXene confirming that there is a direct bonding between OH- and F-terminations to the vanadium atoms on the surface with a water layer bonded to OH-terminations. [117] Although NMR can only detect $^1$H and $^{19}$F atoms on MXenes' surface, its high sensitivity allows direct measurements of bonding and interactions of the surface species. Therefore, advancement in understanding of MXenes' surface chemistry will likely be guided by NMR methods.

Local arrangement of atoms can be determined by neutron/X-ray PDF analysis, comparing calculated PDFs from atomistic models and PDFs resulting from Fourier analysis of diffraction data. One of the advantages of using neutrons over X-rays is that neutrons are sensitive toward hydrogen atoms present on MXenes' surface. However, both methods rely on fitting of experimental data with possible structural models, which could be complicated for MXenes. In an X-ray PDF study, [119] Ti$_3$C$_2T_x$ etched with 50% HF can be best described by a mixture of surface termination with O/F ratio of 0.46. Importantly, this study confirms the spatial positions of the surface terminations to be between three neighboring X atoms (hollow site 1 in Figure 3a) in good agreement with theoretical predictions. In a neutron scattering study (Figure 3g), [118] Ti$_3$C$_2T_x$ etched with 10 and 48% HF concentrations best fit the formula Ti$_3$C$_2$(OH)$_{1.04}$F$_{0.8}$O$_{0.13}$ and Ti$_3$C$_2$(OH)$_{0.8}$F$_{1.1}$O$_{0.1}$ respectively. The surface terminations are distributed randomly as shown in Figure 3h. In good agreement with XPS and NMR studies mentioned earlier, [114,116] the HF-etched Ti$_3$C$_2$T$_x$ MXene contained significantly larger amounts of F- compared to O-terminations. Nonetheless, neutron PDF results showed that there are large amount of OH-terminations in these MXenes, different from XPS and NMR studies. The difference in the content of O- and OH-terminations obtained from the three characterization techniques might stem from the etching environment and sample preparation (e.g., high vacuum of XPS vs ambient environment in PDF analysis) or it might come from the difference in the underlying assumptions and limitations of each characterization technique. Being the only characterization technique that can detect all the possible elements on MXenes' surface, neutron scattering combined with advanced structural modeling PDF could be a promising method to provide insights into MXenes' surface chemistry.

STEM combined with EELS can provide a direct picture of MXenes' surface terminations. Wang et al. showed that the surface terminations are located between three carbon atoms (hollow site 1). [120] This technique is also a useful tool to follow intercalation of other species such as sodium. The limitation of STEM is that it only probes small portions of a sample, so deducing the overall surface termination from this technique can be challenging. Moreover, the sensitivity of STEM toward light atoms such as C, O, and F is limited. EELS can be used to study MXenes' surface at the nanometer scale. Moreover, energy-loss near edge structure (ELNES) of the C and F-K edge can be used to study the hybridization of these atoms with the Ti d-orbitals providing useful information about electronic structure of MXenes. Using C-K edge spectra, Magne et al. suggested that Ti$_3$C$_2$T$_x$ etched by 48% HF or LiF+HCl contained significantly more OH- and F-terminations than O-termination with O/F ratio of 1.4 and 3.5, respectively. [121] Note that this result was deduced from comparing the experimental data with calculations performed without considering mixed surface terminations. Further studies exploiting high-resolution aberration-corrected STEM–EELS analysis could be of importance in understanding MXenes' surface chemistry.

Although Raman spectroscopy has been extensively employed to study vibrational properties of MAX phases, [127,128] there are only a few studies that reported Raman spectra of MXenes. [27,33,112,123,124,129] It was shown that the frequencies and vibrational modes are strongly influenced by surface terminations. [112,129] Moreover, it was shown that in situ Raman spectroscopy can be used to follow protonation of O-termination forming OH-termination in Ti$_3$C$_2$T$_x$ electrode upon discharge in H$_2$SO$_4$ solution. [121] However, precise assignment of Raman modes of MXenes still remains a challenge due to the mixed and random termination species on MXenes' surface.
Moreover, theoretical calculations of vibrational modes were done on monolayer MXene sheets,[112,129,130] while experimental reports on Raman spectra of monolayer MXene have not yet been published. To precisely correlate Raman shifts obtained experimentally to vibrational of surface species, monolayer MXene samples with a well-controlled surface would need to be realized experimentally.

TGA-MS is an efficient tool to study thermal stability of materials, especially desorption of MXenes’ surface terminations. Surprisingly, only a handful of studies reported thermal stability of MXenes’ surface terminations using this technique.[125] Quantification of surface terminations from mass spectra could be difficult due to lack of reference standards for evolved gases. However, TGA-MS serves as an important guide to controlling MXenes’ surface via thermal annealing.[88,131]

Understanding and, ultimately, controlling MXenes’ surface terminations remains one of the most challenging tasks for experimentalists, because many interesting properties are predicted to depend on specific surface chemistry. Since MXenes’ surface is very sensitive to etching conditions and sample preparation, care must be taken when comparing results for MXenes obtained by different synthesis methods. To obtain MXenes with uniform surface termination, post-synthesis treatments must be applied to modify the surface, since wet chemical synthesis always yields mixed surface terminations. Bottom-up synthesis also holds a great promise in producing MXenes with a controlled surface and, ultimately, no surface termination.[108]

4. Computational Studies of Electronic Properties

Electronic properties of MXenes such as metal-to-insulator transition,[110,132] ultralow work function,[111] topological insulator,[57,58,131] large electronic anisotropy,[134,135] and massless Dirac dispersion near the Fermi level[131,136,137] have been extensively investigated computationally. These properties position MXenes among the most studied 2D materials, although most of the properties predicted have not yet been observed experimentally. This part of the review summarizes the theoretical studies and suggests experiments that could be done to verify those predictions.

Nonterminated (bare) MXenes are metallic with a high density of states (DOS) at the Fermi level. However, some MXenes become semiconductors upon surface functionalization (Figure 4a).[35] Semiconducting MXenes and their predicted bandgaps are listed in Table 1. Unless stated otherwise, the bandgap values were obtained using HSE06 hybrid functionals, known to provide relatively accurate estimation of the bandgaps. For most MXenes, the DOS near the Fermi level comprises mainly the transition metals’ d-electrons, whereas the p-electrons of X atoms form energy bands at around −3 to −5 eV below the Fermi level.[110,113] For MXenes, the states near the Fermi level are largely governed by the d-electrons of the metal atoms on the surface. By the same token, the outer transition metal layers (M′) in M2M′XnTx and M′2MXnTx in ordered multielemental transition metal MXenes play a more important role in electronic properties than the M′ inner core metals.[32,61,138,139] This implies that the electronic structure of the surface metals, which can be influenced by the surface functionalization, plays a key role in MXenes’ electronic properties. When the metal surface is terminated, new bands form below the Fermi level, and the Fermi level shifts lower. Importantly, surface functionalization leads to significantly reduced DOS of the surface transition metal at the Fermi level, due to electron transfer from the transition metal to electronegative surface terminations.[79,110,139] With this in mind, OH- and F-terminations are predicted to have similar effect on MXenes’ electronic structure because they can only receive one electron from the surface metal. On the other hand, O-termination might play a different role as it requires two electrons from MXenes’ surface.[110]

Although high electronic conductivity of TiC2T2 makes it promising in many applications, its metallic feature limits its use in switching electronic devices. Despite many predicted MXene semiconductors (Table 1), they have not yet been realized experimentally. Temperature-dependent resistivity measurements of some MXenes show negative slope, dp/dT (typical for semiconductors).[30,61] but the slope changed to positive after annealing, suggesting that the semiconductor-like behavior possibly comes from interflake electron hopping mechanism.[10,88] In search for MXene semiconductors, synthesis and characterization of MXenes with a predicted wide bandgap for all surface terminations, such as Sc2CTx, Cr2CTx, and Cr2TiC2T2 show they should be experimentally realized.[110,132,139] Moreover, control over MXenes surface chemistry is a key to the success in realizing intrinsic semiconducting MXenes. Similar to other 2D materials, electronic band structure of MXenes can be tuned by mechanical strain.[135,141–143] However, effects of strain on MXenes’ electronic properties await experimental verification.

One interesting property of MXenes is that some of them have partially occupied nearly free electron (NFE) states close to the Fermi level (Figure 4b).[144] Such NFE gas layer is located above the hydrogen atoms in the OH-terminated MXenes, such as Hf2TiC2T2 (n = 1–3). Similar observation has been made for OH-terminated Mo2C (where M = Ti, Zr, Hf, Nb, and Ta), Zr2N, and Hf2N. Because the NFE states are located close to the Fermi level, they could be accessible and are anticipated to play an important role in electron transport in nanoelectronics as well as be an active electron donor.[144] Note that the NFE states also exist in other 2D materials such as graphene,[144–146] but those states are much higher in energy and are not easily accessible. Moreover, the NFE states exist at a much higher energy (≈4 eV) above the Fermi level for purely O- and F-terminated MXenes. This, again, emphasizes the importance of the control over surface terminations in order to exploit MXenes’ properties.

Hydroxyl-terminated MXenes were predicted to be ultralow work function electron emitters that are attractive as field emitter cathodes in field effect transistors.[111] More interestingly, MXenes’ work function was predicted to be highly tunable by careful design of a combination of the transition metals, X elements and surface terminations.[111,147] Calculated work functions of M2XTx MXenes are shown in Figure 4c.[111] Generally, the trend in work function follows: O- > F- ≥ bare > OH-terminated MXenes. Among them, Sc2Cl(OH)2 exhibits the lowest work function of 1.6 eV. Because the work function is defined as the difference between the Fermi level and the vacuum level,
naively speaking, shifting the Fermi level to a lower energy upon surface functionalization results in increased work function of O- and F-terminated MXenes. However, this explanation alone is invalid for OH-terminated MXenes because they have lower work function than the bare counterparts. Therefore, there must be another factor that affects the work function, i.e., surface dipole moment ($P$) must be considered. It has been shown that the change in work function ($\Delta \Phi$) is linearly correlated to the change in surface dipole moment ($\Delta P$). For all MXenes studied, OH-termination leads to negative surface dipole moment, and thus decrease in work function.\cite{111} More recent calculations also show that methoxylation of niobium carbide MXenes, Nb$_{n+1}$C$_n$T$_x$ ($n = 1–4$ and T$_x$ = OH$^-$, O$^-$, F$^-$, and CH$_3$O$^-$), led to work function as low as 0.9 eV.\cite{148} Experimentally, the work function of Ti$_2$CT$_x$ thin films was measured by Kelvin probe atomic force microscopy to be ~5.3 eV\cite{149} The authors suggested that their samples were mainly covered by O-termination in their experimental conditions resulting in the high work function. More recent photoelectron spectroscopy measurements of Ti$_2$CT$_x$ thin films showed work function of 4.6 and 4.37 eV\cite{150,151} The difference in the reported values could originate from the variation caused by different measurement techniques or, more probable, the difference in surface terminations. More experimental works on controlling MXenes’ work function by designing their compositions and controlling their surface terminations would be of great importance identifying the ultralow work function materials.

Some MXenes are predicted to be 2D topological insulators (TIs).\cite{57,58,133,136} In this type of materials, the electrons with opposite spins propagate in opposite directions in the edge states resulting in low-dissipation electron transport.\cite{152} They are promising in low-power spintronic devices and quantum computing. The topological edge states are expected in 2D materials with heavy elements, in which spin-orbit coupling (SOC) significantly affects electronic structure.\cite{57} Therefore, MXenes with heavy 4d and 5d transition metals (Mo, W, Zr, and Hf) could exist as 2D TIs. Weng et al. reported that O-terminated M$_2$CO$_2$ (M = W, Mo, and Cr) are 2D TIs with large bandgaps.\cite{136} Due to strong SOC in W$_2$CO$_2$, it exhibits the largest bandgap of 0.47 eV among the other MXenes studied, which renders it promising for practical applications of TIs at room temperature. Independently, Khazaei et al. and Si et al.
metallic ferro- or ferrimagnetic MXenes. In half-
been experimentally synthesized with mixed terminations. The most promising route to experimen-
tations on MXenes' topological behavior. Although none of the
predicted the 2D TI behavior in double-M ordered transi-
tion metal carbides MXenes, M′2M″C2O2 (M′ = Mo, W and
M″ = Ti, Zr, Hf) with O-termination. Shown in Figure 4d
is the local density of states of Mo2HfC2O2. Topologically pro-
cected edge states with a Dirac-cone-like dispersion at the M
point connect the bulk conduction and valence bands. Recently,
Liang et al. showed that the nitride MXene, Ti3N2F2 is a 2D TI,
whereas TI state in Zr3N2F2 and Hf3N2F2 can be induced by
tensile strain. Note that only fully O- or F-terminations have
been considered in all of the studies on topological behavior of
MXenes. There are no reports of the effects of surface termina-
cations on MXenes' topological behavior. Although none of the
predicted MXene TI has been observed experimentally, other
TIIs were predicted first theoretically, and then confirmed by experiments. The most promising route to experimen-
tally realize MXene TIs is to produce and characterize O-termin-
nated Mo2CTx, Mo2TiC2Tx, and Mo2Ti2C3Tx, which have already
been experimentally synthesized with mixed terminations.
In recent years, increasing attention has been given to half-
metallic ferro- or ferrimagnetic MXenes. In half-
metals, one spin channel is metallic, whereas the opposite
spin experiences an energy gap in the spin-polarized density
of states. They are characterized by 100% spin-polarized con-
ducting electrons at the Fermi level. Among many available
transition metals in MXenes, Cr, and Mn-containing MXenes
are the most widely studied ones because they could have large
magnetic moment resulting from half-filled 3d orbitals. Nonterminated Cr2C was predicted to be half-metallic ferromag-
etic with half-metallic gap of 2.85 eV. However, it transformed
to an antiferromagnetic semiconductor with sizable bandgaps
upon surface functionalization. On the other hand, bare
Cr2N is an antiferromagnetic metal and O-functionalization
transformed it to a half-metallic ferromagnet with minority
spin bandgap of 3.88 eV. The calculated current-bias curve also
indicated that Cr2NO2 device exhibits 100% spin-polarized cur-
rent. Different from its carbide counterpart, Cr2NO2 shows
half-metallicity in its surface-passivated form, which could be
obtained relatively easily from experimental perspective. Addition-
ally, it was shown that external strain can induce half-
metallicity in ferromagnetic Cr2C MXene. For Mn-based
MXenes, Mn3CF2 was predicted to be ferromagnetic half-metal
with a bandgap of 2.5 eV. Mn3CF2 could be synthesized from ex-
perimentally available Mn3GaC MAX phase. The challenge
be to selectively etch Ga atoms out from the MAX
phase, producing Mn3CTx with mixed surface terminations,
and then exchange the OH− to O−, and other surface termina-
tions with F atoms. Other predicted MXene half-metal includes
Ti2C,[155] Ti2N,[155] Mo3N2F2,[156] and Ni2NTx (T = F, OH, and O),
transition metals in MXenes, Mn2CF2 was predicted to be ferromagnetic half-metal with a bandgap of 2.5 eV. Mn2CF2 could be synthesized from experimentally available Mn2GaC MAX phase. The challenge would be to selectively etch Ga atoms out from the MAX
phase, producing Mn2CTx with mixed surface terminations,
and then exchange the OH− to O−, and other surface termina-
tions with F atoms. Other predicted MXene half-metal includes
Ti2C,[155] Ti2N,[155] Mo3N2F2,[156] and Ni2NTx (T = F, OH, and O),
W2ZrC2*, O 0.13 [57]
Mo2ZrC2* O 0.13 [57]
Mo2HfC2* O 0.24 [57]
W2TiC2* O 0.29 [57]
W2ZrC2* O 0.28 [57]
W2HfC2* O 0.41 [57]
Hf2MnC2 O 0.24 [138]
Hf2YC2 O 0.06 [138]
Cr2TiC2 F 1.35 [140]
Cr2TiC2 OH 0.84 [140]
Hf2C2 O 0.16 [135]

Table 1. Predicted bandgaps for MXenes with various terminations. Topological insulators are marked by asterisks. The bandgap values reported here were obtained from HSE06 hybrid functionals.

<table>
<thead>
<tr>
<th>MXene</th>
<th>Termination</th>
<th>Bandgap [eV]</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sc2C</td>
<td>O</td>
<td>1.8</td>
<td>[110]</td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>1.03</td>
<td>[110]</td>
</tr>
<tr>
<td></td>
<td>OH</td>
<td>0.45</td>
<td>[110]</td>
</tr>
<tr>
<td>Ti2C</td>
<td>O</td>
<td>0.24</td>
<td>[110]</td>
</tr>
<tr>
<td>Zr2C</td>
<td>O</td>
<td>0.88</td>
<td>[110]</td>
</tr>
<tr>
<td>Hf2C</td>
<td>O</td>
<td>1.0</td>
<td>[110]</td>
</tr>
<tr>
<td>Cr2C</td>
<td>F</td>
<td>3.49</td>
<td>[132]</td>
</tr>
<tr>
<td></td>
<td>OH</td>
<td>1.43</td>
<td>[132]</td>
</tr>
<tr>
<td>Mo2TiC2*</td>
<td>O</td>
<td>0.12</td>
<td>[57]</td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>0.5</td>
<td>[61]</td>
</tr>
<tr>
<td></td>
<td>OH</td>
<td>0.05</td>
<td>[61]</td>
</tr>
<tr>
<td>Mo2ZrC2*</td>
<td>O</td>
<td>0.13</td>
<td>[57]</td>
</tr>
<tr>
<td>Mo2HfC2*</td>
<td>O</td>
<td>0.24</td>
<td>[57]</td>
</tr>
<tr>
<td>W2TiC2*</td>
<td>O</td>
<td>0.29</td>
<td>[57]</td>
</tr>
<tr>
<td>W2ZrC2*</td>
<td>O</td>
<td>0.28</td>
<td>[57]</td>
</tr>
<tr>
<td>W2HfC2*</td>
<td>O</td>
<td>0.41</td>
<td>[57]</td>
</tr>
<tr>
<td>Hf2MnC2</td>
<td>O</td>
<td>0.24</td>
<td>[138]</td>
</tr>
<tr>
<td></td>
<td>F</td>
<td>1.03</td>
<td>[138]</td>
</tr>
<tr>
<td>Hf2YC2</td>
<td>O</td>
<td>0.06</td>
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<td>Cr2TiC2</td>
<td>F</td>
<td>1.35</td>
<td>[140]</td>
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<tr>
<td></td>
<td>OH</td>
<td>0.84</td>
<td>[140]</td>
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<tr>
<td>Hf2C2</td>
<td>O</td>
<td>0.16</td>
<td>[135]</td>
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reported value of as an example) depends strongly on
contact resistance but not the anisotropy of the sample. More
precise conductivity values can be obtained using van der Pauw

5. Experimental Measurements of Electronic and Transport Properties

High electronic conductivity of MXenes makes them promising in many applications, such as EMI shielding, electrode materials in batteries and supercapacitors, transparent conductors, and conductive fillers. Surprisingly, not many in-depth studies on electronic conductivity of MXenes have been reported. As can be seen from Table 2, MXenes' conductivity ranges from less than 1 S cm−1 for a pressed multilayer MXene disc (ML-MXene) to thousands of S cm−1. The reported value of ≈10 000 S cm−1 for Ti3C2T, thin film, which is certainly not the limit. As shown in Figure 5a, MXenes' conductivity (using Ti3C2T as an example) depends strongly on synthesis, delamination, and sample preparation methods. Note that when the conductivity measurements are done on compressed discs, free-standing films, or supported films, MXenes' conductivity is governed by both inter- and intraflake resistance. On the other hand, electronic conduction in single-flake measurements comes solely from intraflake and contact resistance. Electronic conductivity is commonly measured using the linear four-point configuration, which compensates for the contact resistance but not the anisotropy of the sample.
configuration. Generally, use of HF as an etchant leads to smaller, more defective flakes, and higher F-terminations. Therefore, HF-etched multilayer Ti₃C₂Tₓ (ML-Ti₃C₂Tₓ) with random orientation of MXene flakes has a low conductivity of 2 S cm⁻¹ (Figure 5a) possibly due to large interflake resistance, and large intraflake resistance as a result of atomic vacancies and F-terminations that lower carrier concentration at the Fermi level (as discussed in Section 4). The conductivity was improved by an order of magnitude for an ML-Ti₃C₂Tₓ MXene particle, where grain boundary effects vanish. Moreover, vacuum annealing of ML-HF-etched Ti₃C₂Tₓ led to threefold increase in conductivity, possibly due to removal of surface terminations, as will be discussed in the next section. A significant improvement in conductivity was achieved when a mixture of LiF and HCl was used as an etchant. The conductivity of a 5-µm rolled film of ML-Ti₃C₂Tₓ reached 1500 S cm⁻¹. Vacuum-assisted filtered film of delaminated Ti₃C₂Tₓ (d-Ti₃C₂Tₓ) produced by sonication of the LiF+HCl-etched Ti₃C₂Tₓ has conductivity ranging from 1000 to 3000 S cm⁻¹. Higher conductivity values were achieved when Ti₃C₂Tₓ was delaminated without sonication. Free-standing films prepared by such method have the conductivity exceeding 5000 S cm⁻¹. Moreover, conductivity of single-layer Ti₃C₂Tₓ and transparent films prepared by this method reached 6760 and 9880 S cm⁻¹, respectively. Interestingly, thin transparent films trend to exhibit the highest conductivity of all forms of MXene samples, possibly because the film deposition techniques used to prepare transparent films result in well-aligned MXene flakes, minimizing the interflake resistance. When large organic molecules such as DMSO or tetraalkylammonium ions are used in the delamination step, the resulting d-Ti₃C₂Tₓ films show relatively low conductivity, possibly due to suppression of interflake electron hopping.

Temperature-dependent resistivity measurement is a great tool to study transport properties of a material. The results discussed in this section were obtained from stacked d-MXene flakes, so there is an interplay between inter- and intraflake resistance. Ti₃C₂Tₓ MXene showed positive slope of the temperature dependence of resistivity (df/dT), typical for a metal, from 100–300 K. At lower temperatures, df/dT becomes negative (semiconductor-like behavior) as shown in Figure 5b. This behavior is thought to originate from weak localization as supported by negative magnetoresistance (MR) (Figure 5c). We found that the magnitude of this upturn at low temperature depends on synthesis and processing of the samples, which will be discussed in details elsewhere.

In contrast, Mo-based MXene films, i.e., Mo₃CₓTₓ, Mo₂TiCₓTₓ, and Mo₂Ti₂C₃Tₓ exhibited negative df/dT over a temperature range of 10–300 K with positive MR, indicating fundamentally different transport mechanism from Ti₃C₂Tₓ. Although the character of the temperature dependence of resistivity suggests that the Mo-based MXenes could be semiconductors, their behavior could not be described by Arrhenius or variable range hopping (VRH) transport models, with an exception of Mo₂CₓTₓ after annealing. It was shown that post-synthesis heat treatment significantly affects the temperature-dependence of resistivity because of changes in intercalated species as well as surface terminations. Recent in situ EELS study of various MXenes showed that the initially negative slope of the temperature dependence of resistivity, df/dT of the ‘as-prepared’ MXenes can be transformed to a positive value by vacuum annealing, as will be discussed in details in the next section. These results suggest that the electronic conduction of stacked MXene flakes is governed largely by interflake electron hopping process.

To understand intrinsic transport properties of MXenes, electrical measurements must be done on single flakes. However, small lateral size of d-MXene flakes makes fabrication of single-flake MXene devices difficult. Lai et al. reported transport properties of few-layer Ti₃C₂Tₓ prepared by mechanical exfoliation. Monolayer field effect transistor (FET) devices have been successfully fabricated from Ti₃C₂Tₓ. Notably, only etching in LiF+HCl without sonication (MILD method) yields Ti₃C₂Tₓ monolayers that are large enough (up to10 µm) for device fabrication. In all studies, monolayer Ti₃C₂Tₓ exhibited metallic conductivity at room temperature, as can be seen from the linear dependence of source-drain current (I_DS) with source-drain voltage (V_DS). As shown in Figure 5d, Miranda et al. and Lipatov et al. reported that I_DS increased with increasing gate voltage (V_G) indicating that electrons are major charge carriers in Ti₃C₂Tₓ monolayer with field effect mobility of 0.7 and 2.6 cm² V⁻¹ s⁻¹, respectively. Interestingly, Miranda et al. also reported an abrupt change in the I_DS–V_G curve at 2.5 K (Figure 5e), which could be attributed to occupation of a new set of valley band structure with lower mass and/or higher degeneracy. Moreover, increase in resistivity at lower temperature of the monolayer Ti₃C₂Tₓ was attributed to contact resistance rather than weak localization suggested for
Ti$_3$C$_2$T$_x$ thin films. To attain a better understanding of MXenes’ intrinsic electronic properties, further electrical measurements should be done on single flake of Ti$_3$C$_2$T$_x$ and other MXenes. The challenge is to produce MXene monolayer with a large lateral size and high quality.

Like other 2D materials, MXenes exhibit anisotropy of electronic conductivity. MXene layers are separated by a relatively large van der Waals gaps, causing anisotropic properties in the in-plane and out-of-plane directions. The anisotropy was verified experimentally by measuring in-plane and out-of-plane conductivity of an ML-Ti$_3$C$_2$T$_x$ particle (Figure 5f).

It was shown that the in-plane conductivity is an order of magnitude higher than the out-of-plane conductivity. This is because of highly anisotropic band structure with less energy dispersion along the c-axis. Moreover, effective mass of electrons and holes in the basal plane were calculated to be quite small (<0.5 m$_0$), while that of electrons and holes perpendicular to the layers were estimated to be infinite. Moreover, it was shown that the conductivity decreased by fivefold with increasing number of stacked MXene layers from 1 to 9. This highly anisotropic behavior of MXenes could be useful for nanoelectronic devices.

6. Effects of Surface Terminations on Electronic Properties

Surface terminations play an important role in determining MXenes’ electronic properties. While MXenes surface chemistry has been studied extensively computationally, only a handful of experiments have been done to verify its effect on MXenes’ electronic properties. One reason is because producing MXenes with controlled surface terminations is difficult. Furthermore, experimental techniques that can simultaneously follow changes of MXene’s surface and their electronic properties are not widely available.

As discussed in Section 4, electronegative surface terminations decrease DOS close to the Fermi level of MXenes. Therefore, electronic conductivity of terminated MXenes is expected to be lower than that of bare MXenes due to lower charge carrier density. This effect can be seen in an in situ plasma treatment of the Ti$_3$C$_2$T$_x$ thin films. In that study, resistivity of a Ti$_3$C$_2$T$_x$ thin film decreased by 18% when it was treated with low power hydrogen plasma for 10 min (Figure 6a). This change is attributed to removal of OH-terminations.
Moreover, the resistivity increased to the original value when the film was exposed to oxygen plasma, possibly due to formation of O-termination and/or TiO$_2$. Subsequent hydrogen plasma treatment decreased the film's resistivity in a similar manner to the first cycle, showing that surface modification is reversible. A more direct experimental evidence for the effects of surface terminations on MXenes' electronic properties was reported recently by Hart et al.$^{[88]}$ In that study, different MXenes, such as Ti$_3$C$_2$T$_x$, Ti$_3$CNT$_x$, and Mo$_2$TiC$_2$T$_x$, were annealed inside a transmission electron microscope while their electrical conductivity was measured in situ. It was shown by EELS and TGA-MS that MXenes' conductivity increased upon annealing due to deintercalation of adsorbed species and defunctionalization of surface terminations (Figure 6b). When Ti$_3$C$_2$T$_x$ was annealed at the temperature around 100–400 °C, its conductivity increased by almost threefold due to removal of intercalated water and other adsorbed species (improving interflake conductivity), and loss of OH-termination (improving intraflake conductivity). Moreover, the conductivity continued to increase when the sample was annealed up to 775 °C, due to loss of F-termination, as revealed by EELS measurements (Figure 6c). Figure 6d,e shows correlation between reduction of F-and O-terminations with the corresponding conductivity of Ti$_3$C$_2$T$_x$ and Mo$_2$TiC$_2$T$_x$ upon annealing, respectively. Interestingly, only ≈50% of the F-termination was removed even when the sample was annealed at 775 °C under high vacuum (10$^{-7}$ Torr), indicating that F atoms are strongly bonded to the Ti surface. It was further shown that the initial semiconductor-like behavior (negative $\partial \rho / \partial T$) of the as-prepared Ti$_3$CNT$_x$ and Mo$_2$TiC$_2$T$_x$ MXenes changed to metal-like (positive $\partial \rho / \partial T$) when the intercalated species were removed, and the conductivity increased up to tenfold compared to the as-prepared samples. This work demonstrated that surface terminations and intercalated species play an important role in electronic and transport properties of MXenes.

Generally, heat treatment of MXenes in an inert environment leads to a significant increase of conductivity due to removal of intercalated molecules and surface terminations. To better understand the effects of surface terminations on MXenes' intrinsic electronic properties, experimental research should be done on MXene monolayers with controlled surface terminations.

7. Electromagnetic Interference Shielding Properties

High electrical conductivity of MXenes renders them promising in EMI shielding applications, where high conductivity...
is a prerequisite. Electromagnetic interference shielding effectiveness (EMI SE) is directly proportional to materials’ electrical conductivity and thickness, as described by Simon formalism (Equation (4)).[173]

$$\text{EMI SE} = 50 + 10 \log_{10}(\sigma f) + 1.710 \sqrt{\sigma f}$$

where EMI SE is expressed in decibels (dB), $\sigma$ is the electrical conductivity (S cm$^{-1}$), $f$ is the electromagnetic frequency (MHz), and $t$ is the material thickness (cm). Moreover, the total EMI SE is determined from a combination of absorption (SE$_A$), reflection (SE$_R$), and multiple internal reflections (SE$_{MB}$) components. Similar to conventional metals, abundant free electrons at highly conductive MXene surface reflect the incoming electromagnetic wave, while the nacre-like structure of vacuum-filtered MXene films contributes to the multiple internal reflections and absorption. Figure 7a shows electrical conductivity of Ti$_3$C$_2$T$_x$, Mo$_2$TiC$_2$T$_x$, and Mo$_2$Ti$_2$C$_3$T$_x$ films, while Figure 7b shows their corresponding EMI SE from 2.5-µm-thick films. MXene films outperformed other materials of the same thickness in EMI shielding efficiency as shown in Figure 7c.[12] A 45-µm thick Ti$_3$C$_2$T$_x$ film showed EMI SE value of 92 dB, which translates to 99.99999994% EMI blockage in the microwave range. To improve MXenes’ mechanical and environmental stability, reduce weight, and improve processability, they have been incorporated into polymer matrices. Because of their high conductivity and large aspect ratio, MXenes can provide percolation network at a fairly low filler content. As an example, Ti$_3$C$_2$T$_x$/sodium alginate (SA) composites exhibited 0.5 and 3000 S cm$^{-1}$ at 10 and 90 wt% MXene loading, respectively. The 90 wt% composite film with 9 µm thickness showed 57 dB EMI SE.[12] More recent work on

Figure 7. Electromagnetic interference (EMI) shielding properties of MXenes: a,b) Comparison of electronic conductivity (a) and EMI shielding performance (b) of Ti- and Mo-based MXene films. c) Comparison of EMI shielding performance of MXenes and various materials. d) A schematic and e) an SEM image of Ti$_3$C$_2$T$_x$/polystyrene composite formed by electrostatic self-assembly technique. The composites showed improved absorption contribution in the total EMI SE as shown in (f). g) Schematic of Ti$_3$C$_2$T$_x$ MXene integrated into a nanoscale slot antenna arrays. h) Comparison of transmitted terahertz signal between bare Si substrate and MXene nanoarrays. i) Normalized transmittance spectra of 150 nm wide MXene nanoarrays with various thicknesses. a–c) Reproduced with permission.[12] Copyright 2016, American Association for the Advancement of Science. d–f) Reproduced with permission.[174] Copyright 2017, Wiley-VCH. g–i) Reproduced with permission.[184] Copyright 2018, Wiley-VCH.
Ti$_3$C$_2$T$_x$/polymer composites exhibited enhanced electrical conductivity due to their dielectric nature. In the latter study, relatively high conductivity at low MXene content was achieved possibly due to the electrostatic assembly approach used to prepare the composites as shown in Figure 7d. Indeed, the percolation threshold was achieved at 0.26 wt%, much lower than other MXene/polymer composites.\textsuperscript{[163,175]} An SEM image of the Ti$_3$C$_2$T$_x$/PS composite is shown in Figure 7e, indicating that PS microspheres were wrapped together by MXene sheets. EMI SE of the composites is shown in Figure 7f. One way to improve EMI properties of MXene/polymer composite is to use a conductive polymer matrix to provide both mechanical support and electrical conduction. Tong et al. reported in situ chemical oxidative method to prepare Ti$_3$C$_2$T$_x$/polyaniline (PAni) composites, and showed that a 3 mm thick film of 25 wt% composite exhibited 49.2 dB reflection loss (≈99.99% absorption).\textsuperscript{[176]} The EMI SE of the Ti$_3$C$_2$T$_x$/PPy composites could be improved if oxidation of MXene could be minimized during polymerization step, which can be achieved via oxidant-free polymerization technique.\textsuperscript{[177]} Additionally, other conducting polymers have been reported to form composites with Ti$_3$C$_2$T$_x$ MXenes,\textsuperscript{[178,179]} which could be interesting for EMI shielding applications. More recently, Cao et al. reported MXene/cellulose nanofiber composite paper with EMI SE ≈25 dB from a 74 μm thick paper with 80 wt% MXene loading. The composite paper exhibited improved mechanical properties with 135 MPa tensile strength.\textsuperscript{[180]} MXene composites with other active EMI absorbers such as carbon nanotubes (CNTs), zinc oxides, and hexagonal barium ferrites were also reported.\textsuperscript{[181–183]} Ti$_3$C$_2$T$_x$ integrated into nanoscale slot antenna arrays was found to have enhanced EMI SE in the terahertz (THz) range.\textsuperscript{[184]} The device was fabricated by drop-casting of delaminated Ti$_3$C$_2$T$_x$ solution onto a prepatterned Au nanoslot antenna array on Si substrate as depicted in Figure 7g. MXene suppressed the THz transmission when integrated into a nanoray with 150 and 500 nm wide antennae (Figure 7h). Moreover, the fundamental resonances of the nanoantenna at 1 THz vanished when the MXene thickness reached 65 nm, and the transmitted intensity decreased by two orders of magnitude with 1 μm thick MXene film. The THz transmission was significantly suppressed over 0.5 to 2.0 THz range, in agreement with theoretical predictions, showing that Ti$_3$C$_2$T$_x$ is a good absorber in the terahertz range.\textsuperscript{[185]} Furthermore, the effects of thermal annealing on dielectric and EMI shielding properties of Ti$_3$C$_2$T$_x$ were reported by Han et al.\textsuperscript{[186]} It was shown that annealing of HF-etched Ti$_3$C$_2$T$_x$ MXene at 800 °C in Ar atmosphere led to formation of TiO$_2$ nanoparticles, and amorphous carbon supported on the remaining MXene flakes. The thermal annealing provides additional contribution to EMI shielding performance due to higher electronic conductivity and lower permittivity of both carbon and TiO$_2$ formed on MXene surface. The dielectric loss and EMI SE of the 1.7 mm thick 50 wt% Ti$_3$C$_2$T$_x$/wax composite after annealing are ~48.4 and 32 dB, respectively. Porous structures could potentially be beneficial for EMI shielding applications due to increased internal reflection.\textsuperscript{[187]} Liu et al. reported fabrication of hydrophobic porous Ti$_3$C$_2$T$_x$ foam via hydroxy-induced foaming process.\textsuperscript{[188]} The resulting porous foam exhibited EMI SE of ~70 dB, and its hydrophobicity improved its environmental stability.

Counterintuitively, the main contribution in EMI SE comes from absorption component rather than reflection component as expected from materials with metal-like high electron density at the surface. Luo et al. proposed that reflection loss observed in Ti$_3$C$_2$T$_x$-filled paraffin composites stems from a combination of “microdipole” relaxation loss within MXene sheet and hopping migration loss between MXene sheets.\textsuperscript{[189]} Similar mechanism was proposed for Ti$_3$C$_2$T$_x$/PPy composites.\textsuperscript{[176]} More work is needed to completely understand the mechanism of EMI shielding of MXenes and, in general, other 2D materials to have a control over the absorption and reflection components. Although other MXenes showed a lower electrical conductivity than Ti$_3$C$_2$T$_x$ so far, their diverse compositions may lead to interesting light-matter interaction and they deserve further study.

8. Sensors

8.1. Pressure and Strain Sensors

MXenes have been used as pressure and strain sensors by virtue of their electrical response to strain caused by an external force.\textsuperscript{[16–18,190]} The main mechanism in MXenes’ pressure sensors is piezoresistive, where external pressure is transduced into a change in resistance signal. Reasonably, MXene’s conductivity increases (decreases) when the interlayer spacing shrinks (expands). This phenomenon was reported by Hu et al., where more than 10 times increase in the out-of-plane conductivity was reported for an ML-Ti$_3$C$_2$T$_x$ particle with applied pressure.\textsuperscript{[134]} Recently, Ma et al.\textsuperscript{[16]} reported that ML-Ti$_3$C$_2$T$_x$ can be used as a pressure-sensitive layer in a pressure sensor (Figure 8a). It was demonstrated that the device’s current output, which is governed by MXene’s conductivity, increased monotonically with increasing pressure with high Gauge Factor (GF) of 180 and fast response time of less than 30 ms.\textsuperscript{[16]} Strain from 0.19–2.1% was detectable with high precision. The response of MXene’s interlayer space to applied pressure was illustrated by in situ dynamic process inside a TEM (Figure 8b), showing working mechanism for the piezoresistive sensor. Moreover, it was also demonstrated that this MXene pressure sensor could be used to detect human movement, such as joint bending and breathing as shown in Figure 8c. The same group has also shown that MXene/reduced graphene oxide (GO) aerogel had sensitivity of 22.56 kPa$^{-1}$ toward external strain over 10 000 cycles. The aerogel also showed low detection limit of 10 Pa, which is suitable for detection of human pulse.\textsuperscript{[191]} Improvement in sensing performance was achieved with a d-Ti$_3$C$_2$T$_x$/carbon nanotubes (CNTs) composite sensor as shown in Figure 8d.\textsuperscript{[177]} The sensing layer was fabricated by alternate spray-coating of d-Ti$_3$C$_2$T$_x$ and aqueous solution of single-walled CNTs on a latex substrate. The resulting composites exhibited mechanical resilience and could be stretched to 200% strain without failure (Figure 8e). Figure 8f shows the piezoresistive response of the composite with the applied strain varying from 0 to 80%. At low strains (0–30%), the composite exhibited GF of 64.6, whereas the GF value increased to 772 at high strains (40–70%). Moreover, the composite showed stable performance for more than 5000 cycles. Unlike the previous MXene sensor works where...
the change in conductivity stemmed from the change in interlayer spacing of ML-Ti$_3$C$_2$T$_x$, the response of d-Ti$_3$C$_2$T$_x$/CNTs composites results from sliding of d-MXene flakes and CNTs, disconnecting the conductive pathways. Therefore, the d-Ti$_3$C$_2$T$_x$/CNTs sensor conductivity decreases with external pressure. Composites of d-Ti$_3$C$_2$T$_x$/PVA hydrogel with more than 3400% stretchability were recently reported (Figure 8g). The hydrogel exhibited GF of 25 and 80 under tensile and compressive strain, respectively. More interestingly, it showed anisotropic electrical response to the direction of strain, where its conductivity decreased (increased) under tensile (compressive) strain as shown in Figure 8h. This phenomenon was attributed to the alignment of the 3D network structure of MXene nanosheets inside the hydrogel matrix, where the compressive strain reduces the gaps between MXene sheets, resulting in an increase of the composite’s conductivity (Figure 8i).[18]

A more recent work has shown that layer-by-layer assembly of Ti$_3$C$_2$T$_x$/poly(diallyldimethylammonium chloride) on flexible polymeric substrate showed decrease in conductivity upon bending and stretching due to formation of microcracks on MXene surface. Interestingly, the cracks and gaps recover upon release of external pressure, reforming conductive pathways and allowing the device to work for thousands of cycles.[190]

MXene-based pressure sensors attracted much attention recently due to their outstanding performances and fairly easy device fabrication. To further improve sensing performance of MXene pressure sensors, material choice and design of the composite/foam architecture must be accomplished. Although effects of strain engineering on MXenes’ band structure alignment have not been studied experimentally, high sensitivity pressure sensors could be achieved from a strain-induced metal-to-insulator transition in MXene-based devices.
8.2. Molecular Sensing

High sensitivity of MXenes’ conductivity to adsorbed species and abundant adsorption sites on their functionalized surface make MXenes highly attractive for molecular sensing applications. Theoretically, it has been shown that semiconducting M\textsubscript{2}CO\textsubscript{2} (M = Sc, Ti, Zr, and Hf) are highly sensitive to NH\textsubscript{3} adsorption (Figure 9a). Calculations showed that adsorption of NH\textsubscript{3} leads to charge transfer from NH\textsubscript{3} molecules to the transition metal atoms on MXene surface, causing increase in MXenes’ electronic conductivity (Figure 9b,c).

Moreover, it was shown that NH\textsubscript{3} molecules can be desorbed from MXene surface upon electron injection in to the MXene layer, making the sensors reusable. This happens because of the special characteristic of MXenes’ electronic states, where the DOS close to the Fermi level come primarily from the metal atoms. Thus, the injected electrons spread mainly on the transition metal, resulting in increase in the NH\textsubscript{3}-metal bond length and adsorption energy, and thus making it less energetically favorable for the NH\textsubscript{3} to adsorb on MXene surface. Another study has also shown that Sc\textsubscript{2}CO\textsubscript{2} is sensitive to SO\textsubscript{2} gas. Charge transfer from SO\textsubscript{2} to Sc\textsubscript{2}CO\textsubscript{2} leads to large increase in DOS at the Fermi level and several orders of magnitude increase in MXene’s electronic conductivity.

Recent computational study has shown that O-terminated M\textsubscript{2}C (M = Ti, V, Nb, and Mo) could be used in gas sensing applications with Ti\textsubscript{2}CO\textsubscript{2} and Nb\textsubscript{2}CO\textsubscript{2} being more sensitive to NH\textsubscript{3}, while Mo\textsubscript{2}CO\textsubscript{2} and V\textsubscript{2}CO\textsubscript{2} being more sensitive to NO. Interestingly, it was shown that charge transfer from adsorbates to bare MXenes surface may lead to dissociation of the adsorbate molecules, making MXenes promising catalysts for small molecule activation.

Despite intensive computational studies on MXene gas sensors, only a few experiments have been reported on the subject. Separately, Lee et al. and Kim et al. reported on the...
use of Ti$_3$C$_2$Tx for sensing of volatile organic compounds (Figure 9d).\[15,196] The former study showed that Ti$_3$C$_2$Tx gas sensing device could detect as low as 100 ppm polar gases, such as ethanol, methanol, acetone, and ammonia, at room temperature. The lowest detection limit of 25 ppm was achieved for acetone. It was also shown that the original resistance of the device was recovered upon desorption of gases, except for ammonia, indicating strong bonding between ammonia and Ti$_3$C$_2$T$_x$ surface.\[196] In another study, as low as 50 ppb acetone concentration was detected at room temperature.\[15] In addition, Ti$_3$C$_2$Tx was shown to be more sensitive toward volatile organic gaseous compounds compared to acidic gases such as NO$_2$ and SO$_2$, as shown in Figure 9e. In contrast to the previous work where the gas sensor was more sensitive toward ammonia among other gases, the sensor reported by Kim et al. showed the highest sensitivity toward ethanol with gas response of 1.7% at 100 ppm concentration.\[15] Moreover, the increase in MXene’s resistance upon gas adsorption was attributed to reduction of charge carriers of the metallic conduction channel. DFT simulations predicted that MXene’s surface terminations strongly affect binding energy of different gases with Ti$_3$C$_2$O$_2$(OH)$_2$ forming the strongest bonds with both ammonia and acetone, as shown in Figure 9f. It is worth mentioning that an increase in MXene’s resistance upon gas adsorption was observed in both experimental studies, in contrast to computational predictions.\[192,193] This might be due to the metallic nature of Ti$_3$C$_2$Tx used in the experimental studies as opposed to semiconducting MXenes studied computationally. One possible explanation for increase in devices’ resistance with gas adsorption might be that the adsorbed gas molecules increase spacing between MXene sheets and suppress inter- flake electron hopping processes. Actual gas sensing mechanisms of MXenes need further study to better understand the interactions between MXenes and adsorbate molecules. Monolayer MXene may also be a good candidate for producing high-performance gas sensing devices.

MXene was also exploited in biological sensing. As an example, FET based on Ti$_3$C$_2$Tx was used for dopamine and neural activity detection, as shown in Figure 9g.\[197] Interestingly, the device showed gate-dependent ambipolar characteristic (Figure 9h), and the conductivity of the device increased with increasing dopamine concentration, possibly due to hole-doping effect of dopamine (Figure 9i).\[198] The device showed a large detection range of $1 \times 10^{-7}$ to $2 \times 10^{-3}$ molar dopamine concentration. Moreover, MXene also exhibited excellent biocompatibility and stability in neural activity measurements despite an anticipated high F content on the surface.

MXenes have also been employed as substrates for other functional materials for sensing applications. For example, stimuli-responsive poly[2-(dimethylamino)ethyl] methacrylate polymer was grafted onto V$_2$CT$_x$ MXene. The composite was sensitive to temperature fluctuation and CO$_2$ adsorption.\[199] Hemoglobin-immobilized on Ti$_3$C$_2$T$_x$ particles was sensitive toward H$_2$O$_2$ and nitrite detection.\[200,201] Glucose oxidase enzyme immobilized on Nafion solubilized Au/MXene nanocomposite can be used as a glucose biosensor.\[202] MXene/DNA/Pd/Pt nanocomposite was shown to have high sensitivity and selectivity toward dopamine detection.\[203] Recently, partially oxidized Ti$_3$C$_2$T$_x$ thin films were reported to show a photoresponse in the UV region due to TiO$_2$ nanocrystals formed on conductive MXene sheets.\[204]

It is important to note that sensing applications of MXenes is based on changes in either electrical, electrochemical, or optical properties with external stimuli. Therefore, understanding the underlying mechanisms of the effects of stimuli on the aforementioned properties of various MXenes is an important step toward exploiting them in sensing applications.

9. MXene Heterostructures

The 2D nature of MXenes allows them to be assembled, layer-by-layer, with other MXenes or 2D materials forming van der Waals heterostructures with precisely chosen sequence as shown in Figure 10a.\[205,206] Theoretical studies have shown that the electronic properties of MXenes are greatly affected by heterostructure formation.\[207-211] Because of a close lattice match between MXenes and transition metal dichalcogenides (TMDs), MXene/TMD heterostructures have been extensively studied theoretically and experimentally.\[93,106,207,208,210] A DFT study has shown that MoS$_2$ forms a chemical bond with bare Ti$_2$C surface with induced metallic character in the DOS of MoS$_2$ as shown in Figure 10b.\[207] In contrast, the interaction at the MoS$_2$ and surface-terminated Ti$_2$CT$_x$ interface is described as weak physisorption. Interestingly, MoS$_2$/Ti$_2$CT$_x$ heterojunction formation leads to n-type doping of the MoS$_2$ layer resulting from electron transfer from metallic MXene with Schottky barrier height of 0.85 eV and 0.26 eV for MoS$_2$/Ti$_2$CF$_2$ and MoS$_2$/Ti$_3$C(OH)$_2$, respectively. The effects of n-type doping could be beneficial for electron-donating applications of MoS$_2$, e.g., catalyst for hydrogen evolution reaction. In addition, Schottky barrier height can be tuned by band engineering of the metal/semiconductor interface to align metal’s work function with the semiconductor’s band edges, which is feasible due to MXenes’ tunable work functions as shown in (Figure 8c.).\[147] DFT calculations suggested that OH-terminated MXenes can form electron barrier-free contact with 2D semiconductors, e.g., WS$_2$. Moreover, many O-terminated MXenes such as Ti$_3$C$_2$O$_2$, Mo$_x$CO$_2$, V$_2$CO$_2$, and V$_2$NO$_2$ can form hole barrier-free contact with WS$_2$.\[147] Recent calculations also showed that some MXenes can form heterojunctions with blue phosphorene, a 2D allotrope of phosphorus, with small lattice mismatch and negative binding energies. Similar to MoS$_2$, strong interaction between blue phosphorene and bare MXenes leads to induced-metallic character in the band diagram of the former. When MXenes are surface-terminated, the interaction is much weaker and blue phosphorene preserves its semiconducting behavior. It was shown that the electron barrier vanished in blue phosphorene/M$_{x}$Ti$_{1-x}$C$_{2}$Tx (M = Zr, Hf and T = OH, F) and Nb$_{x}$Ta$_{1-x}$C$_{2}$O$_{2}$ heterostructures.\[212] The same group also showed that O-terminated Zr$_x$CO$_2$ and Hf$_x$CO$_2$ form type-I heterostructures with blue phosphorene that can be transformed to type-II heterostructures by tensile strain.\[143] The semiconductor/semiconductor heterostructures will be discussed later in this section. More recently, effects of doping and surface functionalization on electronic and transport properties of M$_2$CT$_x$/M$_2$CO$_2$ (M = Ti, Zr, and Hf) were also reported.\[213]
Experimentally, Ti$_2$CT$_x$ with work function of 4.98 eV was used as a source electrode in n-type MoS$_2$ and p-type WSe$_2$ FET devices (Figure 10d,e). The electron and hole barrier height were estimated to be 0.19 and 0.23 eV for the MoS$_2$ and WSe$_2$ devices, respectively. Considering the high work function of Ti$_2$CT$_x$ and small electron barrier height, strong Fermi level pinning effect is expected at the MXene/MoS$_2$ interface. The electron barrier height estimated for MoS$_2$/Ti$_2$CT$_x$ is close to that of MoS$_2$/Ti$_2$C(OH)$_2$ predicted computationally. Moreover, a complementary metal oxide semiconductor (CMOS) inverter, where the n- and p-type FETs are linked together sharing a common gate electrode (Figure 10f), was fabricated and showed signal inversion with a gain of 3.4. Ti$_3$C$_2$T$_x$/n-type silicon (n-Si) heterostructure has been shown to be a self-driven photodetector with a $I_{\text{photo}}/I_{\text{dark}}$ of 10$^5$ and 27 mA W$^{-1}$ responsivity (Figure 11c). Strong built-in electric field ($V_d$) near the Ti$_3$C$_2$T$_x$/n-Si interface separates photoinduced carriers generated under illumination with Schottky barrier height of 0.74 eV as shown in Figure 11a,b. The device’s performance could be optimized by varying MXene’s thickness to minimize contact and sheet resistances while maintaining sufficient transparency. Work function of the Ti$_3$C$_2$T$_x$ electrode could be modified by thermal annealing, resulting in the change in Schottky barrier height and device’s performance. Using metallic MXenes as electrodes is promising in nanoelectronic device applications because MXene work function can potentially be tuned to match with the semiconductor’s band edge by selecting MXene’s compositions and controlling their surface terminations. However, synthesis of large-area MXene monolayers with high purity remains a challenge. Contaminations trapped between MXene flakes and/or...
metal/semiconductor interface are known to negatively affect the device’s performance. Moreover, control and analysis of monolayer MXenes’ surface terminations remain challenging.

Semiconductor/semiconductor heterostructures are interesting in a way that they provide tunable electronic band properties according to the type of heterojunction formed. MoS2 and M2CO2 (M = Ti, Zr, Hf) formed a type-II heterostructure, where the bandgaps of the two materials are staggered with valence band maximum and conduction band minimum located on different layers as shown in Figure 12a. For example, formation of MoS2/Zr2CO2 heterostructure resulted in an indirect bandgap of 0.28 eV, which is much different from the original properties of the two materials (2.13 eV direct bandgap and 1.62 eV indirect bandgap in MoS2 and Zr2CO2, respectively), demonstrating that large varieties of band properties can be achieved through band engineering. With partial charge transfer from Zr2CO2 layer to MoS2, holes and electrons are accumulated on the former and the latter layers, respectively, inducing a built-in electric field. The resulting built-in field and indirect bandgap character can help with spatial charge separation, which is useful in photocatalytic applications. It was also predicted that semiconductor-metal transition can be introduced at 1.5% strain. Similarly, type-II heterostructures with variable bandgaps are formed when Sc2CF2 is stacked with MoS2, MoSe2, WS2, and WSe2. More interestingly, various kinds of heterostructures can be produced from all-MXene combinations by pairing different MXenes (Figure 12b).

Particularly, type-I heterostructure is formed when stacking Sc2CF2 and Sc2CO2 together, while type-III heterostructure is formed when stacking F- and -OH or O- and OH-terminated Sc2CTx together. Modification of surface terminations’ positions resulted in different types of heterostructures as shown in Figure 12c,d. Equibiaxial strain induced transformation of the heterojunctions to form type-II heterostructures as shown in Figure 12e. Thus, all types of heterostructures could be achieved using the same MXene base by varying surface terminations, stacking interface, and strain.

There are numerous possible combinations of MXenes and other 2D materials to form heterostructures with useful properties. Several MXene heterostructures for energy storage and other applications have been studied computationally and experimentally. CVD is a promising synthesis route to obtain high-quality 2D heterostructures, but it has not yet been applied to MXenes.

10. Optoelectronic Properties: Transparent Conductive Thin Films

High electrical conductivity, 2D morphology, processability, and excellent mechanical properties render MXenes promising candidates for transparent conductors. Several film deposition techniques including magnetron sputtering, spray-coating, electrospaying, spin-casting, dip-coating, and interfacial film
assembly have been reported to produce Ti$_3$C$_2$T$_x$, Ti$_2$CT$_x$, and V$_2$CT$_x$ transparent thin films.[13,14,71,149,164,218–222] The first transparent MXene film was produced via etching of magnetron-sputtered Ti$_3$AlC$_2$ MAX phase deposited on sapphire substrate (Figure 13a). This is the only top-down method among the aforementioned film deposition techniques. The resulting films exhibited transmittance of 14–85% with conductivity $\approx 2000$–5000 S cm$^{-1}$. Interestingly, the MAX phase is also transparent in the visible light, although it absorbs more light compared to the corresponding MXene with the same thickness. Moreover, it was observed that films made with large intercalants, i.e., NH$_4^+$ ions, were more transparent and less conductive than those with small interlayer spacing, possibly due to expansion of the c-lattice parameter.[71] UV–visible spectra (Figure 13a) show a clear difference between that of MAX and MXene, where the former has relatively flat spectrum from 200 to 1000 nm range while latter has strong absorption around 300 nm and a broad absorption around 800 nm. Using solution-processing techniques, such as spray-coating, spin-casting, or dip-coating, transparent MXene films with different thicknesses can be deposited on glass or flexible substrates as shown in Figure 13b,c. The cross-sectional SEM image shows that MXene flakes align parallel to the substrate’s surface resulting in compact conductive layer. Spin-casting is believed to yield high-quality transparent films with well-aligned MXene flakes due to centrifugal shear force produced during high-speed spinning. The optical quality Ti$_3$C$_2$T$_x$ films reached conductivity of 6600 S cm$^{-1}$ while remaining >97% transparent, corresponding to figure of merit of 5 (FoM = $\sigma_{DC}/\sigma_{opt}$ where $\sigma_{DC}$ and $\sigma_{opt}$ are electronic and optical conductivity, respectively). As shown in Figure 13d, the percolative conduction path was formed at the sheet resistance value of 1000 $\Omega$ sq$^{-1}$ implying low percolation threshold at 2 nm thickness. Interestingly, the real part of optical permittivity ($\varepsilon_1$) becomes negative at wavelength $>1130$ nm indicating the onset of free-electron plasma oscillations (Figure 13e). Notably, the Ti$_3$C$_2$T$_x$ films show strong absorption in the near-IR region (Figure 13c) with the onset wavelength similar to the negative $\varepsilon_1$ in permittivity measurement. These results are in good agreement with DFT predictions.[223] It was found that the film’s conductivity increased by threefold after storage in dry N$_2$ atmosphere. Moreover, vacuum-annealing of the films was shown to significantly improve their conductivity, while maintaining the films’ transparency.[149] Therefore, drying the films after deposition is one way to achieve high FoM. Thin films prepared by spin-casting using nonsonicated d-Ti$_3$C$_2$T$_x$ and vacuum-annealed at 200 °C showed the highest conductivity of MXene reported so far, 9880 S cm$^{-1}$, with a corresponding FoM of 15.[164] Additionally, Ti$_2$CT$_x$ thin films on flexible substrate showed a slight decrease in conductivity upon bending to small radii, and stable conductivity during bending cycles, as illustrated in Figure 13f. Spin-cast Ti$_2$CT$_x$ films were reported to have FoM of 0.5 and 5 by different groups.[164,218] The high FoM value of the Ti$_2$CT$_x$ films in the latter work might partly come from Ti$_3$C$_2$T$_x$ present in the d-MXene dispersion used for deposition. The 312 and 211 phases often coexist in the MAX precursor, as described in reference 72.[72] Despite several advantages of spin-casting technique, high concentration d-MXene dispersion (usually $>5$ mg mL$^{-1}$) is needed.
to obtain considerably thick films.\textsuperscript{218,224} Moreover, the substrate must be flat and the substrate size is limited by the spin chamber, which limits large-scale production of MXene thin films. On the other hand, spray-coating method provides a simple and scalable thin film deposition alternative. Thin films of Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} MXene can be deposited on a large area with controllable thickness from solution with a relatively low concentration (0.5–3 mg mL\textsuperscript{−1}).\textsuperscript{[13]} A large range of film thicknesses from a few nanometers to micrometer-thick film can be fabricated by repeating the spraying process.\textsuperscript{[225]} This method is also applicable to fabrication of MXene/metal oxide hybrid composites.\textsuperscript{[167]} Interestingly, it was shown that the films’ transparency could be tuned by chemical and electrochemical intercalation of organic and inorganic cations making Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} a promising candidate in electrochromic application.\textsuperscript{[13]} Electrospaying technique can also be used to deposit low-concentration MXene solution. The resulting thin films, however, had rough surface with obvious grain boundaries.\textsuperscript{[219]} Dip-coating has been used to prepare Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} thin films with high quality. It was shown that plasma treatment of the deposited films not only improved film’s conductivity, possibly by removing surface oxides, but also decreased the film thickness as a result of layer-by-layer etching.\textsuperscript{[221]} Recently, V\textsubscript{2}CT\textsubscript{x} thin films were prepared by spin-casting using colloidal suspensions with tetrabutylammonium hydroxide (TBAOH) as a dispersant. Notably, the ‘as-prepared’ films had sheet resistance in the range of 10\textsuperscript{5}–10\textsuperscript{6} Ohm sq\textsuperscript{−1} and it decreased by two orders of magnitude after annealing, possibly due to TBAOH decomposition. The V\textsubscript{2}CT\textsubscript{x} films showed absorption coefficient of 1.2 × 10\textsuperscript{5} cm\textsuperscript{−1}, which is more than twice as transparent as Ti-based MXene films reported.\textsuperscript{[222]}

Fabrication of MXene transparent thin films makes it possible to study their fundamental electronic and optical properties, which will be discussed in the following sections. To meet a requirement of transparent electrodes, FoM of more than 30 is needed (commercially available indium tin oxide has FoM \approx 200).\textsuperscript{[226]} Higher film conductivity could be achieved by improving MXene flake size and quality, deposition techniques, and post-deposition treatment. Further, most of the works reported to date focus on Ti-based MXenes in aqueous solution, while optoelectronic properties of other MXenes remain unexplored. Moreover, effects of surface terminations, ion intercalation, and/or solvents on films’ quality, electronic conductivity, and optical properties should be investigated.

\section*{11. Nonlinear Optical Properties}

Nonlinear optics deals with the light-matter interaction in the regime where materials nonlinearly respond to electromagnetic field. This phenomenon is crucial for applications such
as laser optics, photonic devices, and optical communication. Only recently that nonlinear optical properties of MXenes have been demonstrated.\textsuperscript{220,227–229} \textbf{Z-scan} measurements (Figure 14a,b) show that Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} exhibits nonlinear light absorption (saturable absorption, SA), viz., the transmission increases nonlinearly with increasing illuminating intensity. Typically, effective nonlinear absorption coefficient decreases with increasing illuminating intensity until a threshold intensity ($I_{th}$) as shown in Figure 14c. The nonlinear absorption coefficient of Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} was found to be $-10^{-21}$ m$^2$ V$^{-2}$, indicating potential use in optical switching applications.\textsuperscript{228} This behavior is believed to stem from plasmon-induced ground state absorption when Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} MXene is illuminated by a laser with the wavelength comparable to its plasmon resonance frequency.\textsuperscript{229} As evidenced from a peak in the imaginary component of dielectric constant ($\varepsilon_2$) and a crossover in the real component ($\varepsilon_1$) at wavelengths of 800 and 1130 nm, respectively, where the former is assigned to surface plasmon resonance and the latter is assigned to free-carrier oscillation.\textsuperscript{144} Similar plasmonic behavior was also observed by an electron energy loss spectroscopy study.\textsuperscript{210} Interestingly, SA was observed at different illuminating wavelengths from 800 to 1800 nm, suggesting that there might be more than one mechanisms contributing to nonlinear absorption behavior of Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x}.\textsuperscript{228} For Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x}, it was proposed that one-photon process saturable absorption dominates at low illuminating intensity, while multiple-photon absorption process occurs at higher illuminating intensity, and the other nonlinear absorption processes become the dominant mechanism at the laser intensity above $I_{th}$.\textsuperscript{228} SA ability of MXenes enables them to be used in ultrafast laser applications. For this application, MXene serves as a spectral filter that induces mode-locked laser pulses. Metallic Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} and Ti\textsubscript{3}CNT\textsubscript{x} were used in femtosecond mode-locked lasers as shown in Figure 14d.\textsuperscript{227,228} Figure 14e,f shows that Ti\textsubscript{3}CNT\textsubscript{x} produced stable mode-locked laser pulses with a period of 65 ns and temporal width of 660 fs.\textsuperscript{227} Similar performance was obtained for Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x}.\textsuperscript{228} The broadband wavelength from 1550 to 1620 nm produced by Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} covers the essential telecommunication band (C-band) indicating a promise in communication applications. The nonlinear optical performance of MXenes is comparable, if not superior, to other 2D materials such as transition metal dichalcogenides, graphene, and black phosphorus.\textsuperscript{228} Moreover, it was shown that Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} with a thickness of 5 nm is more resilient at high laser energy than other 2D materials.\textsuperscript{228} It was further demonstrated that Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} can be coupled with C\textsubscript{60}, a reverse saturable absorption material, forming an optical diode.\textsuperscript{220} The device could be used to filter optical signal with a high rectification ratio. Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} was also shown to produce random lasing when dispersed in rhodamine 101 solution, forming a metamaterial.\textsuperscript{231} Studies of nonlinear optical properties of MXenes are still in the early stage, yet have already shown promise in many applications. Interaction of light with MXenes needs further systematic investigations. Photonic, optoelectronic, and plasmonic properties of different MXenes await further exploration before practical applications.
12. Plasmonic Properties

Ti$_3$C$_2$Tx exhibits attractive plasmonic properties and holds a promise for use in surface-enhanced Raman spectroscopy (SERS) application.[27,28,121,230,232] EELS analysis has shown that multilayered Ti$_3$C$_2$Tx has intense surface plasmons with energy range from 0.3 to 1 eV that dominate over bulk plasmons even at 45 nm layer thickness.[230] This result is in good agreement with spectroscopic ellipsometry data obtained from a 75 nm thick film.[14] This peculiar behavior of MXene is unique unlike other plasmonic materials such as gold nanoparticles, in which the surface plasmon vanished when the particle size exceeded 30 nm.[233] It was also shown that the bulk plasmon peak is independent of the layer thickness, unlike other 2D materials where the bulk plasmon peak blueshifts when going from few layers to bulk state.[234] Moreover, MXene’s electronic structure, which is greatly affected by surface terminations, is believed to influence surface plasmon resonance.[223,230,232] Therefore, it is possible to tune MXenes’ plasmonic behavior by modifying their surface terminations. Because of the surface plasmonic nature of Ti$_3$C$_2$Tx, it acts as a high efficiency SERS substrate with enhancement factor (EF) of $10^6$, allowing detection of Rhodamine 6G organic dye at $10^{-7}$ molar (Figure 15a,b).[27] The enhancement mechanism was attributed to charge transfer from MXene substrate to dye molecules. Moreover, it was demonstrated that Ti$_3$C$_2$Tx can be used as a substrate for noble metal nanoparticles in SERS application.[235] Another application exploiting surface plasmon properties of MXene is metamaterial absorber.[28] Nanodisk arrays of Ti$_3$C$_2$Tx were fabricated on various substrates as shown in Figure 15c. It was demonstrated that absorption and reflection spectra of MXene can be tuned by varying the disks’ diameter and substrates. The device with the disk diameter of 450 nm on Au/Al$_2$O$_3$ showed increased absorption over a broad range of UV–visible–NIR spectra, as shown in Figure 15d. This result shows that electromagnetic wave absorption, especially in the NIR range, of MXene can be greatly improved via nanostructure design of MXene arrays, enabling surface plasmon resonance scattering. This nanostructured MXene device is promising in energy harvesting (light-to-heat conversion application), biomedical

![Figure 15](https://www.advancedsciencenews.com/advmat/article-pdf/30/25/1804779/1804779.pdf)

**Figure 15.** Plasmonic properties: Ti$_3$C$_2$Tx MXene exhibits plasmonic property that is suitable for surface-enhanced Raman spectroscopy (SERS) and metamaterial absorber applications. a) A schematic of SERS substrate made from Ti$_3$C$_2$Tx MXene. b) Raman spectra of Rhodamine 6G dye collected on the MXene SERS substrate. c) SEM images of microfabricated Ti$_3$C$_2$Tx MXene nanodisk arrays. Scale bars are 1 µm in all images. d) Absorption spectra of the Ti$_3$C$_2$Tx arrays showing improved absorption in a wide electromagnetic wavelength. a,b) Reproduced with permission.[27] Copyright 2017, American Chemical Society. c,d) Reproduced with permission.[28] Copyright 2018, American Chemical Society.
imaging, and sensing applications. Nonetheless, little is known about plasmonic and photonic properties of MXenes, and their respective applications need further investigation. Nitride and carbonitride MXenes are expected to show more pronounced surface plasmon-related phenomena similar to bulk transition metal nitrides. Synergistic efforts from both modeling and experiments are needed to further explore plasmonic and photonic properties of MXenes.

13. Light-to-Heat Conversion and Photothermal Therapy Applications

Another important property of MXenes that has been investigated only recently is light-to-heat conversion and its use in photothermal therapy. Typically, MXenes showed relatively high extinction coefficient ($\varepsilon$) around 15–40 L g$^{-1}$ cm$^{-1}$, comparable if not higher than that of other photoabsorbing materials such as Au nanorods, GO, and reduced graphene oxide (rGO). As shown in Figure 16a, MXene flakes can absorb and convert light energy to heat energy when a laser is shone through a droplet of MXene colloidal solution. From this experiment, Ti$_3$C$_2$T$_x$ MXene exhibits light-to-heat conversion efficiency ($\eta$) close to 100%, where temperature of the MXene solution droplet increased by 17 $^\circ$C within a minute of laser illumination (Figure 16b). The increase in solution temperature depends on the absorption coefficient, droplet size of the MXene solution, and is directly proportional to MXene concentration and laser illumination power. Due to different experimental setups reported in the literature, it is difficult to compare light-to-heat conversion performance based on the increase in the solution temperature alone. It is, therefore, recommended that light-to-heat conversion efficiency ($\eta$) is used to compare performance of different MXenes. Despite strong absorption in the UV region of most MXenes, UV illumination has not been used to study their light-to-heat conversion properties. More than 200% increase in extinction coefficient is expected comparing the near-infrared (NIR) and UV regions based on the UV–visible spectroscopy results.

Because of its high light-to-heat conversion efficiency, Ti$_3$C$_2$T$_x$ also shows excellent performance in photothermal steam generation. Shown in Figure 16c is the water evaporation rate of Ti$_3$C$_2$T$_x$ films prepared by vacuum-assisted filtration of MXene solution with different mass loading. It was shown that water evaporation rate increases with increasing MXene loading. The film with 10 mg mass loading yielded water evaporation efficiency of 74% compared to 30% evaporation efficiency in the absence of MXene film. Moreover, it was shown that the

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**Figure 16.** Light-to-heat conversion and photothermal therapy applications: high optical absorption of MXenes renders them promising in light-to-heat conversion and photothermal therapy applications. a) A schematic experimental setup for light-to-heat conversion experiment. b) Temperature profile of d-Ti$_3$C$_2$T$_x$ droplet when illuminated by different lasers. c) Water evaporation rate of MXene membrane under one sun irradiation. d) Confocal fluorescence images of breast cancer cells before and after Ti$_3$C$_2$T$_x$ photothermal treatment. The live and dead cells are labeled with green and red staining, respectively. e) Cells viabilities after treatment with different concentrations of Ti$_3$C$_2$T$_x$, MXene. f) Infrared thermal images of tumor-bearing mice with and without Ti$_3$C$_2$T$_x$ injection under 808 nm laser irradiation. a–c) Reproduced with permission. Copyright 2017, American Chemical Society. d–f) Reproduced with permission. Copyright 2016, American Chemical Society.
efficiency can reach 84% when a polystyrene heat barrier was incorporated on the back side of the membrane.\textsuperscript{[247]}

Several MXenes, including Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x}, Nb\textsubscript{2}CT\textsubscript{x}, Ta\textsubscript{4}C\textsubscript{3}T\textsubscript{x} and their composites have been shown to be efficient photothermal therapeutic materials. MXenes show high absorption coefficient in a wide range of wavelengths in both visible and NIR regions, which is particularly suitable for photothermal therapy applications. Although d-MXene can be dispersed in water and other polar solvents without obvious aggregation,\textsuperscript{[105]} they are not necessarily stable in physiological solutions. Therefore, their surface was further modified by soybean phospholipid (SP) or polyvinylpyrrolidone (PVP) to improve their colloidal stability. It has been shown that SP-modified Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} can be dispersed in several common physiological media and remains photothermal-active.\textsuperscript{[238]} Moreover, large organic intercalants such as tetrapropylammonium hydroxide and prolonged sonication were used to delaminate MXenes to obtain small flakes, suitable for transport through cell membranes. For in vitro studies, surface-modified MXene flakes were injected into tumor cells, followed by NIR laser illumination. It was shown by confocal laser scanning microscopy results (Figure 16d) that significant amount of the cancer cells were killed after photothermal treatment (marked with red color) as compared to the control group (marked with green color). It was also shown in Figure 16e that MXene-treated cancer cells without laser illumination were still viable up to 100 µg mL\textsuperscript{-1} MXene concentration, showing that MXenes have negligible cytotoxicity effects on the 4T1 cancer cells, consistent with another study.\textsuperscript{[246]} Shown in Figure 16f are IR thermal images of tumor-baring mice with or without intravenous Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} injection under 808 nm laser irradiation. It was shown that mice with MXene injection developed increase in tumor surface temperature up to 60 °C after 10 min of illumination, and the tumor was completely eliminated without recurrence within the observation period.\textsuperscript{[238]} It was also shown that MXene intake showed negligible effects on mice’s body weight, behavioral change, and the key biochemistry parameters. Moreover, PVP-modified Nb\textsubscript{2}CT\textsubscript{x} can be decomposed by human myeloperoxidase after 24 h of incubation.\textsuperscript{[239]} These results suggest that MXenes deserve further in vivo cancer therapy studies. It was further demonstrated that MXene composites with transition metal oxides showed improved performance in photothermal therapy. For example, MnO\textsubscript{x}/Ta\textsubscript{4}C\textsubscript{3}T\textsubscript{x} and Fe\textsubscript{2}O\textsubscript{3}/Ta\textsubscript{4}C\textsubscript{3}T\textsubscript{x} composites not only exhibited photothermal and superparamagnetic properties (for iron-containing MXene composites), but can also be used for X-ray computed tomography and as a magnetic resonance imaging contrasting agent.\textsuperscript{[240,244]} Finally, it was shown that chemotherapy agents (anticancer drugs) can bind with MXene surface to improve stimuli-responsive drug release and tumor-specific accumulation, creating a theranostic platform based on MXenes.\textsuperscript{[243,247]}

High-efficiency light-to-heat conversion ability of MXenes has already attracted great attention and been used in photothermal therapy applications. Although it has been shown that Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x} MXene have negligible cytotoxicity to human cells and mice, MXene production requires the use of toxic chemicals such as HF and tetraethylammonium hydroxide. Toxicity of other MXenes should be systematically studied. Careful cytotoxicity evaluation must be done before their clinical translation. Moreover, MXenes a with larger absorption coefficient in the NIR region are to be identified for improved photothermal therapy performance.

### 14. Conclusions and Perspectives

Here, electronic and optical properties as well as related applications of MXenes have been reviewed. This large and rapidly growing family of 2D transition metal carbides, carbonitrides, and nitrides has been demonstrated to exhibit attractive electrical, optical, electrochemical, and mechanical properties, which lead to numerous applications. A large variety of transition metals and surface terminations provide endless opportunities to tune the compositions and properties of MXenes. Combination of hydrophilic surface and large negative zeta potential make them highly dispersible in water and polar organic solvents, and thus ideal for solution-processing.

High electronic conductivity resulting from conductive transition metal carbide/nitride core layers enables applications of MXenes in EMI shielding, transparent conductors, electrodes for high power energy storage devices, and conductive fillers. Ti\textsubscript{3}C\textsubscript{2}T\textsubscript{x}, the first and most studied MXene, has the highest conductivity reaching 10 000 S cm\textsuperscript{-1} in thin films. MXenes’ electronic conductivity depends on etching and delamination methods as well as post-synthesis treatments. Strong response of MXenes’ conductivity to external stimuli renders them promising for pressure, light, and molecular sensors. The 2D nature of MXenes allows them to form van der Waals heterostructures with other 2D materials with interesting electronic band properties. Exploiting their optical and plasmonic properties, applications such as ultrafast lasers, optical communication, SERS substrates, metamaterial broadband absorber, and light-to-heat conversion have been realized. Particularly, there is a growing interest of using MXenes in photothermal therapy applications.

Despite several years of extensive research on MXenes, our understanding of this exciting family of materials is still at an early stage. Many of their fundamental properties remain unexplored. For example, the nature of their surface terminations is still under a debate. Synthesizing MXenes with a uniform surface termination remains one of the most important and challenging tasks for experimentalists. Ultimately, MXenes with no surface termination must be synthesized by vapor phase deposition in vacuum or other methods. Moreover, intrinsic MXene semiconductors have not yet been experimentally realized, despite DFT predictions. Experimental measurements of their electronic band structures and the effects of surface terminations as well as oxidation states of the transition metals on the band structure have not been reported. Several exciting properties such as topological insulators, superconductivity, and half-metallicity have been predicted by DFT; and await experimental confirmation. Several MXenes are predicted to exhibit strong magnetization even at room temperature, which is appealing for 2D spintronics. Optical properties of MXenes are very attractive. However, the mechanisms of interactions of MXenes with electromagnetic waves are poorly understood, while they are of critical importance for use in EMI shielding, photonics, and plasmonic applications.

To further advance our knowledge and understanding of MXenes’ properties, synergistic efforts from theory and experiments are needed. Experimentally, high-quality MXene
flakes with large lateral dimension (preferably, >30 μm), fewer defects, and controlled surface termination must be synthesized. To achieve this goal, minimally invasive etching and delamination methods should be developed for all available MAX and non-MAX precursors. Nonfluorinated etchants that can effectively produce MXenes with high yield are particularly attractive, especially for biomedical applications. Moreover, size-selection methods should be developed to obtain MXene flakes with controlled flake sizes and thicknesses. Chemical modifications and/or heat treatment protocols must be developed to obtain uniform surface terminations. Moreover, synthesis of new MAX and other layered carbide and nitride precursors with high quality and large crystal size is important for expanding the MXene family. Mixed surface terminations should be used in calculations to reflect the true composition of MXenes and predict their properties with higher accuracy. Additional theoretical studies focusing on electronic, optical, and magnetic properties of MXenes are needed to provide insights into experimental results and further guide experiments. Recently, it was shown that machine learning can predict bandgaps of MXenes with high accuracy. In the foreseeable future, machine learning will play an important role in predicting MXenes’ properties.

We hope that this review will serve as a guide to those exploring electronic and optical properties of MXenes and help reduce the gap between theoretical predictions and experimental observations. We would like to point out that the experience accumulated in studies of fundamental electronic, optical, and magnetic properties of graphene, transition metal dichalcogenides, and other 2D materials should be applied to MXenes. It is time to advance our understanding of those properties of MXenes and identify the most promising applications for this family of 2D materials.

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Conflict of Interest
The authors declare no conflict of interest.

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