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Two-dimensional MXenes and their applications

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Two-dimensional (2D) transition metal carbides, nitrides or carbonitrides (MXene) have attracted tremendous attention as a potentially the largest family of inorganic materials. They have a general formula $M_{n+1}X_nT_x$, where M is an early transition metal (2 or more can be present in a random mix or a specific order), X is C and/or N elements (oxygen can partially substitute), and T_x (x is variable) represent surface terminations, which can include reactive end groups (such as –OH and =O), halogens and chalcogens, and n can vary from 1 to 4 (fractions are possible). All MXenes can either be produced as multilayer particles (*ml*-MXene) or delaminated (*d*-MXene) single-layer flakes.

Their superior properties and numerous application prospects are the ones to credit for the ever-increasing attention to this family of materials since the first report on $Ti_3C_2T_x$ MXene published in 2011 [1]. Typical MXenes combine metallic conductivity of transition metal carbides and nitrides with hydrophilic and redox-active surfaces that occur as a result of their hydroxyl or oxygen terminations. One can look at them as metallically conductive clays or water dispersible/processable 2D metals with a tunable density of states at the Fermi level. This perspective article is a part of the special topic of *Frontiers of Physics* on MXene and Its Applications. It particularly addresses research topics covered by the journal.

Given this unique combination of properties of MXenes, there are numerous promising applications that are being explored, which include lithium and sodium-ion batteries [2], supercapacitors [3], electrocatalysts nanomaterials [4], optoelectronic devices [5], and flexible sensors [6], to name a few. In particular, this special topic of *Frontiers of Physics* includes papers on such novel and important topics as MXene-based bifunctional oxygen electrocatalysts for rechargeable zinc–air battery [4] and a polarization-sensitive, self-powered, broadband and fast $Ti_3C_2T_x$ MXene photodetector covering the range from visible to near-infrared and driven by the photogalvanic effect [5].

In parallel with the increasing number of MXene structures and compositions reported, the proportion of different applications in the total number of MXene publications has changed drastically over the past decade. The chart in Fig. 1(a) that is based on our Web of Science search with different topics on 31 December 2022 shows more than 12 500 MXene publications. Moreover, further analysis shows an order of magnitude increase in the total number of MXene publications since the end of 2018 [Fig. 1(b)]. Another interesting aspect is the expansion of MXenes to new research fields, such as mechanical engineering, biomedical engineering, and electronics, particularly flexible and printable electronics, as well as optoelectronics. It is noteworthy that Alshareef and co-workers suggested a term MXetronics for MXene-based opto-electronic devices and nanosystems [7]. The increase in the proportion of new research fields in the total number of MXene publications is partially attributed to rapid successful applications of MXenes in those new fields, but biomedical and energy-related applications keep rapidly expanding too.

With the rapid development of modern microelectronics and telecommunication, 2D MXene materials, their derivatives and van der Waals heterostructures, could be used to design microwave absorbers with predefined and tunable properties [8, 9]. In particular, the next generation of wearable electromagnetic interference (EMI) shielding materials requires flexibility, lightweight, ultrathin and

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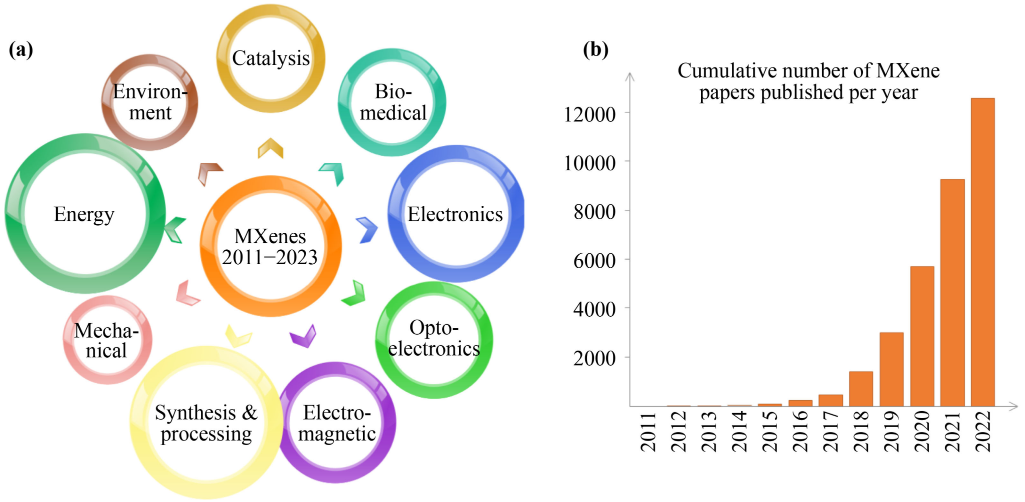

Fig. 1 Explored applications and properties of MXenes to date. **(a)** The circle chart shows the ratio of publications in different application of MXenes with respect to the total number of publications on MXenes [30]. **(b)** The bar chart shows the cumulative number of MXene publications per year.

robustness to protect microelectronic devices from electromagnetic radiation pollution. Flexible and ultrathin dopamine modified MXene@cellulose nanofiber (DM@CNF) composite films with alternate multilayer structure have recently been produced by a facile vacuum filtration induced [9]. Oxygen electrocatalysts are of great importance for the air electrode in zinc–air batteries (ZABs). Owing to large surface area, high electrical conductivity and ease of modification, the elaborately modified 2D MXene-based electrocatalysts exhibit excellent performance toward the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER). Motivated by the rapid development of bifunctional electrocatalysts toward ORR and OER, Ma and co-workers reviewed the latest progress of electrocatalysts based on MXenes, graphene and other 2D materials, covering structure, synthesis, and electrocatalytic performance of these catalysts, as well as their applications in rechargeable ZABs [4]. The article also addresses the challenges in the field and provides outlook for advancing the rechargeable ZABs.

MXenes are typically prepared from MAX phase ceramic precursors by selectively etching A-element (usually, Al) layers [1, 6]. The crystal structure of MAX phases is comprised of $M_{n+1}X_n$ structural units and the single atomic planes of A stacked alternately. Notably, the MAX phases and their derived MXene phases have both metal features and ceramic features, and they are anticipated to be promising thermoelectric materials. When reaching the monolayer limit, it is often that the crystals start to behave very differently comparing to their 3D counterparts [10]. Interestingly, some MXenes are predicted to have distinct magnetic properties, such as ferromagnetic order with a range of transport behaviors, including metallicity, half-metallicity, and semimetallicity [11–14]. Recently, ferromagnetism [12–15] has been predicted and superconductivity experimentally confirmed [16] in 2D MXene materials. Particularly, out-of-plane ordered *o*-MXenes with the formulas $(M'_2M'')X_2T_x$ and $(M'_2M''_2)X_3T_x$, where M'' atoms constitute the inner metal layer(s), and M' atoms are placed in the outer layer (e.g., $Cr_2TiC_2T_x$) are promising [14]. Chromium containing *o*-MXenes $Cr_2M''CT_x$ (T = H, O, F, OH, or bare), where M'' = Sc, Y, Ti, Zr, Hf, V, Nb, Ta, Mo, or W, have been predicted to achieve intrinsic magnetism by spin-polarized density functional theory (DFT) calculations, which provides a new comprehensive potential strategy for designing MXenes in spintronics. It is worthwhile highlighting that ferromagnetic half-metallicity, antiferromagnetic semiconducting, as well as antiferromagnetic half-metallicity have been predicted in the *o*-MXenes [15]. What's more, ferromagnetic half-metallic Cr_2ScC_2, $Cr_2ScC_2H_2$, $Cr_2ScC_2F_2$, and $Cr_2YC_2H_2$ are characterized with wide band gaps and high Curie temperatures. In addition, the antiferromagnetic semiconducting Cr_2TiC_2, Cr_2ZrC_2, and $Cr_2ZrC_2(OH)_2$, have been predicted to possess moderate band gaps and high Neel temperatures. Antiferromagnetism and switchable ferromagnetic/antiferromagnetic states in MXenes have also been predicted [13, 14]. As a consequence, due to the unmatched chemical and structural diversity of MXenes, new physics is being discovered in MXenes, covering a variety of functional properties in semiconducting, half-metallic, semimetallic, and metallic states [11, 12, 16].

Due to the unique electronic structure of half-metals, it is expected that the half-metallicity 2D MXene materials may emerge as a suitable alternative for the design of efficient giant magnetoresistive (GMR) devices. Based on the first-principles calculations, an excellent GMR device has been designed by using 2D half-metal Mn_2NO_2[17]. Mn_2NO_2 MXene sandwiched between the Au/$n$$Mn_2NO_2$ (n = 1, 2, 3)/Au heterojunction is expected to maintain its half-metallic properties. Due to the half-metallic characteristics of Mn_2NO_2, the total current of the monolayer device can reach up to 1500 nA in the ferromagnetic state. At low voltage, the maximum GMR is observed to be 1.15×10^{31} %. This computationally designed spintronic device exhibits the highest magnetoresistive ratio reported theoretically so far [17]. It is concluded that, due to its excellent half-metallic properties and 2D structure, Mn_2NO_2 is an ideal energy-saving GMR material. Of course, experimental realization poses a challenge, but the community is now aware of potentially attractive properties and a very important application for this still-to-be-made MXene. It means that attempts will be made to make it in the lab. Meanwhile, it is further found that a significant negative differential resistance (NDR) effect is also observed in the Au/$n$$Mn_2NO_2$ (n = 1, 2, 3)/Au heterojunction [17]. Note that the heterojunction fabrication generally requires the use of molecular beam epitaxy (MBE) or chemical vapor deposition (CVD) technologies in order to precisely control the atomic deposition thickness and create a high-quality lattice-matched heterojunction interface. A recent alternative is the stacking of exfoliated 2D materials into van der Waals heterostructures, and moreover, formation of such atomically thin heterostructure, or combinations with other nanostructures to form heterojunctions, can be used, for instance to develop novel semiconductor transistors and/or photodetectors [18, 19]. At this point, the field of semiconductor optoelectronics is dominated by heterojunction devices, and probably the dominant effect, when assembling van der Waals heterostructures for nanoscale devices, is the charge transfer due to difference in the work function of the adjacent crystals. In MXenes, the work function can be finely tuned between 2 and 6 eV by controlling their surface chemistry [3]. Besides, it is very likely that the van der Waals heterojunction would further result in many more exciting phenomena to study and improved or even fundamentally new devices for applications. On the other side, since the optical properties are related to their band structures, MXenes are promising for various optoelectronic applications, especially in all-optical modulators and photodetectors, due to metallicity with a chemically tunable Fermi level or a small band gap (less than 0.2 eV) and broadband saturable absorption capability [20]. Additionally, the performance of metal-anchored 2D materials originates from the unsaturated coordination state of the active center and the strong interactions that are stable in physical examination [21]. Meanwhile, optical switches using layered materials have attracted considerable interest in recent years. Ultrafast all-optical switching was demonstrated in graphene due to its strong optical nonlinear absorption with a switching time of 260 fs [22]. As a comparative study, by probing the dynamics of carriers in short-time intervals, Zhang *et al.* [23] recently designed nanoengineered 2D MXene by anchoring Au nanoparticles with a size of 3–5 nm on the surface to study ultrafast all-optical switching. Moreover, the determinant of the energy transfer between the plasmonic metal nanoparticles and the $Ti_3C_2T_x$ MXene substrate is the generation of high-energy electron-hole pairs excited by local surface plasmon resonance (LSPR). The LSPR excitation induces ultrafast transmission and broadband differential transmission, which can be employed as a tunable switch integrated in optical communication systems and integrated circuits. According to experimental transient absorption spectra of Au/MXene and pure MXene, the Au/MXene couple exhibits a better performance with an emerging switching of 290 fs (FWHM) in the near-infrared (NIR) region with the switching red-shift of 34 nm, demonstrating that the Au/MXene hybrids are promising for application in optoelectronics [23].

Apart from the all-optical modulators and ultrafast optical switches, a key device for optoelectronic applications is a photodetector, for which self-powering, broadband detection, and polarization sensitivity are desirable physical qualities. Currently, only very few photodetectors can fulfill these requirements simultaneously. Xie *et al.* [5] have recently proposed a $Ti_3C_2T_x$ MXene photodetector that is driven by the photogalvanic effect with impressive performances. A polarization-sensitive photocurrent is generated at zero bias under the illumination by linearly polarized laser source of 1064 nm, with an extinction ratio of 1.11. Meanwhile, a fast response with a 32/28 ms rise/decay time and a large on/off switching ratio of 120 were achieved. Besides, a robust zero-bias photocurrent was also generated in the photodetector under the 940 nm and 620 nm illumination, as well as the white light, showing a broadband photoresponse from the NIR to visible. Based on quantum transport simulations, it is inferred that the photogalvanic effect plays an important role in the generation of the polarized photocurrent at zero bias due to the broken space inversion symmetry of the stacked few-layer MXene. These results further shed light on potential applications of MXenes in optoelectronics, particularly in the high-performance photodetection.

In recent years, various MXenes and MXene derivatives with outstanding electrical and mechanical properties, flexibility, and high sensitivity have been introduced into the field of flexible and/or wearable sensors for potential applications in health monitoring [6, 24, 25], motion detection [6, 24, 25], human-machine interaction [26], and artificial intelligence [6, 27]. Particularly, MXene-based hydrogels have drawn significant attention. For example, inspired by biomineralization, multifunctional MXene mineral hydrogels have been produced [24].

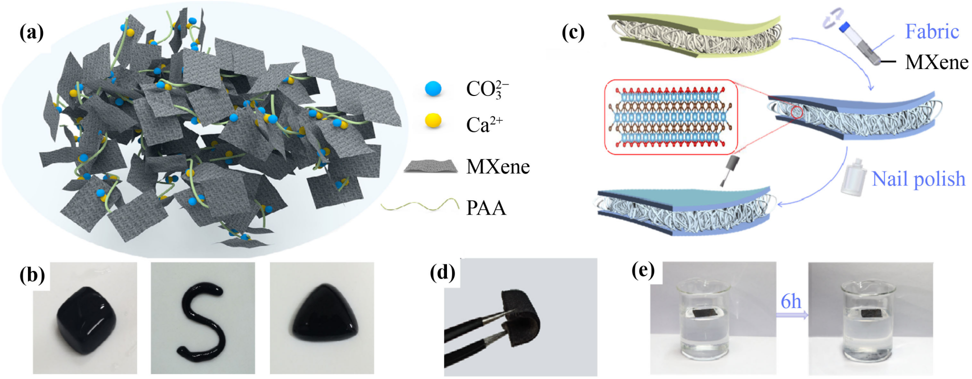

Fig. 2 Architecture of the MXene-based mineral hydrogel and textile. **(a)** Schematic image of the MXene-based mineral hydrogel (reproduced from Ref. [24]). **(b)** The MXene-based mineral hydrogel made into different shapes. **(c)** Schematic diagram for fabrication of the MXene-based textile sensor. **(d)** Image illustrating the flexibility of the MXene-based textile. **(e)** Image illustrating the initial state when the MXene-based textile placed in water and its unchanged shape after immersion for 6 hours.

As shown in Figs. 2(a) and (b), the prepared MXene mineral hydrogels were self-healable, stretchable and conductive, and could be used to fabricate wearable strain sensors directly attached to human skin. They can detect tiny and large human motions, exhibiting a super-wide sensing range with excellent sensitivity. This method is simple and cost-effective, easy to transition into large-scale production and does not require complex processes or additional packaging, showing promise in wearable healthcare monitoring equipment, intelligent robots and efficient human-machine interfaces.

Furthermore, there have also been some studies on MXene-based textile electronics for detecting human pulse, respiration, body movement, etc. [28, 29]. However, imparting excellent mechanical and electrical properties while maintaining the wearing comfort has been a great challenge because most of them need to be attached to the skin with tapes or band-aids. MXene-based textile electronic devices, being flexible, are particularly promising for human health and motion monitoring because of their softness, portability, and air permeability [29]. As schematically shown in Fig. 2(c), a flexible MXene-based textile pressure sensor fabricated by assembling MXene onto the scuba knit with a hollow structure exhibits multiple sensing properties, such as high pressure sensitivity (GF = 23.7 kPa^{-1}), very good stability, and excellent waterproof capability after 6 h immersion in water, as shown in Fig. 2(e). Additionally, a personalized intelligent health monitoring system integrated with the MXene-based textile sensors has been developed to collect and analyze physiological signals from different people at multiple time periods, demonstrating a great advance in wearable health monitoring.

The MXene research community is continuing to make progress, as many of the challenges listed in Ref. [29] are being tackled and several have been resolved in the past three years. Notably, MXenes with uniform surface terminations have been realized, scalable and fluorine-free synthesis methods developed, high-entropy MXenes with 3 to 5 transition metals and oxycarbide MXenes have been added to the MXene family [30, 31]. In addition, many new members of the MXene family, abundant derivatives of MXene materials and MXene-based van der Waals heterostructures have emerged with attractive, often unique, properties and promising applications. Computational studies have predicted many exciting properties in already synthesized MXenes and in the ones that are still being studied in the lab. These predictions will certainly stimulate synthesis of new MXenes and further expansion of this family, which may include more than a thousand stoichiometric compounds and an infinite number of solid solutions. Future efforts should focus not only on synthesis and characterization of new MXenes but also on design and fabrication of heterostructure devices and developing MXene architectures. Those efforts will add to ever-growing practical applications of MXenes in energy, electronics, communications, environmental and healthcare fields.

Declaration of competing interest The authors declare no competing financial interests.

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