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MXenes

Cutting-Edge Materials for
Next-Generation Applications

Edited by Tianzhu Zhou



MXenes - Cutting-Edge Materials for Next- Generation Applications

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Aims and Scope of the Series

Materials science has always occupied an extremely high position in the human development process. As we explore the oceans of stars, various industries have put forward more stringent requirements for the performance of materials, forcing us to pay more and more attention to the development of new materials. At the same time, the formation of a data-driven scientific paradigm is dramatically shortening the development cycle of new materials. The huge data generated by synergistically combining theories, high-throughput experiments, high-throughput computation, and artificial intelligence is greatly contributing to our ability to utilize materials science to solve real-world problems. The three topics of this book series - Metals and Nonmetals; Composite Materials; and Surface Science - will address important areas of advancement in materials science. There will be a range of interesting works published under these topics.

Meet the Series Editor



Prof. Chonghe Li received his Ph.D. from the Chinese Academy of Sciences in 1995. From 1995 to 2000, he worked as a researcher at the Shanghai Institute of Metallurgy, Chinese Academy of Sciences, where he also served as director of the research laboratory. In 2000, he was appointed Professor at the Institute of High-Performance Computing in Singapore, where he worked on computation and simulation in materials science until 2004. Since then, he has been a professor at the School of Materials Science and Engineering, Shanghai University, China, as well as the director of the Shanghai Specialty Casting Engineering and Technology Research Center. Prof. Li's research focuses on titanium alloys, titanium-aluminum single crystals, intermetallic compounds, theoretical calculations, alloy design, and special refractory materials. His broad scientific expertise is well recognized by the scientific community around the world. He is a member of the editorial board of the journal *Metals*. As an author, he has published more than 200 peer-reviewed papers, 2 books, and over 40 patents.

Meet the Volume Editor



Dr. Zhou is currently a professor at the University of Science and Technology of China (USTC). He earned his Ph.D. from Beihang University (BUAA) in Beijing, China. Dr. Zhou was a Research Fellow at Nanyang Technological University, Singapore. Dr. Zhou's research focuses on scalable fabrication of strong, tough, and smart fibers and their application in wearable textiles for energy conversion, biomedicine, and artificial intelligence. In recent years, Dr. Zhou has made significant contributions to his field, publishing over 20 papers in prestigious international journals in Science, Nature Communications (3), PNAS, Science Advances, Advanced Materials, and Angewandte Chemie International Edition (2). He has also authored two book chapters and holds six authorized invention patents, including two international PCT patents.

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Preface

MXenes, a rapidly expanding family of two-dimensional transition-metal carbides and nitrides, have attracted significant attention over the past decade due to their unique combination of electrical conductivity, tunable surface chemistry, mechanical flexibility, and solution-processability. These attributes position MXenes as a versatile materials platform capable of bridging fundamental science and practical technologies. The present book aims to provide a focused and coherent overview of recent progress in MXene research, with particular emphasis on structure-property relationships, device-relevant performance, and emerging applications in electronics, computing, biomedicine, and energy storage.

Chapter 1 introduces MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) nanosheets integrated into fiber-assembled nanocomposites, highlighting how their layered structure and surface-functionalized chemistry can be leveraged during assembly. The chapter reviews synthesis strategies, mechanical and electrical properties, and interfacial interactions, with particular attention to the role of interfacial engineering in tailoring composite performance. Key applications in flexible sensors, energy storage, photothermal conversion, and biocompatible devices are discussed, illustrating the potential of MXene-based fiber nanocomposites as foundational materials for wearable and flexible electronics.

Chapter 2 addresses the growing demand for energy-efficient and data-intensive computing driven by the rapid development of artificial intelligence. This chapter provides a comprehensive overview of MXene-based flexible neuromorphic memristor devices as a potential solution to the limitations of conventional von Neumann architectures. Material engineering strategies for MXene thin films, classifications of MXene-derived neuromorphic materials, and their switching mechanisms are systematically discussed. Advances in memory devices, artificial synapses, neuromorphic circuits, and in-sensor computing are analyzed, followed by an outlook on remaining challenges and opportunities for MXene-enabled sensing-memory-processing systems.

Chapter 3 focuses on the biomedical applications, where MXene-based composite materials are emerging as promising candidates for next-generation healthcare technologies. This chapter summarizes recent advances in combining MXenes with polymers, metal nanoparticles, and carbon-based materials to enhance biocompatibility, stability, and multifunctionality. Applications in drug delivery, cellular imaging, cancer therapy, tissue engineering, sensing, and antimicrobial treatments are reviewed, along with a critical discussion of current challenges and future research directions in translating MXene composites toward practical biomedical use.

Chapter 4 examines the fundamental electrical properties of titanium carbide ($\text{Ti}_3\text{C}_2\text{T}_x$) MXene, with an emphasis on solution-processed thin films. The chapter explores how synthesis routes, flake quality, surface terminations, and film thickness influence electrical conductivity, which spans several orders of magnitude. The dual

charge transport mechanisms, band-like conduction within individual flakes and thermally activated hopping between flakes, are discussed in detail. This contribution underscores the importance of structural and morphological optimization for achieving reproducible, high-performance MXene films suitable for electronic applications.

Chapter 5 focuses on the role of surface-terminated MXenes in advancing the safety and performance of metal-ion batteries through intrinsic thermal management. The chapter reviews recent progress in tailoring MXene surface terminations to achieve high electrical conductivity and low infrared emissivity, thereby reducing heat generation and thermal radiation during fast charging and discharging. Experimental and computational insights are presented to elucidate how engineered terminal groups enable flexible electrodes with self-thermal management capabilities, highlighting the broader significance of surface-functionalized two-dimensional materials in next-generation energy storage technologies.

The chapters in this book reflect the interdisciplinary nature of MXene research and demonstrate how advances in synthesis, characterization, and interface design translate into functional devices and systems. We hope this book will serve as a valuable reference for researchers, engineers, and students working in materials science, physics, chemistry, and related fields, and inspire further innovation in the development of MXene-based technologies.

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Chapter 1

Interface-Engineered MXene Fibers for Flexible Electronics

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Zhenkai Chen, Tianzhu Zhou and Qunfeng Cheng*

Abstract

MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) nanosheets are increasingly being incorporated into fiber-assembled nanocomposites, leveraging their distinctive layered architecture, excellent electrical conductivity, and remarkable mechanical properties, including tunable surface moiety chemistry used in flexible electronics. This chapter reviews recent advances in MXene-based fiber nanocomposites, covering synthesis strategies, mechanical and electrical characteristics, interfacial behavior, and emerging applications. It examines how interfacial engineering facilitates the integration of MXene into fibrous networks and tailors the functional performance of the composites. The discussion also highlights critical uses of these materials in flexible sensors, energy storage systems, photothermal conversion, and biocompatible devices. These multifunctional fiber nanocomposites have shown significant potential across various domains, providing a robust platform for the advancement of wearable and flexible electronics.

Keywords: interface-engineered strategies, MXene nanosheets, fibers, mechanical and electrical properties, flexible electronics

1. Introduction

As research continues to advance, the fiber-based nanocomposites fabricated from two-dimensional (2D) nanosheets have emerged as a key area of advanced materials research, playing a significant role in accelerating the development of flexible wearable technologies [1]. Nano-materials such as graphene nanosheets, MXene nanosheets, black phosphorus nanosheets, and transition metal dichalcogenide nanosheets exhibit a set of common and distinctive properties [2–5], which allow them to demonstrate remarkable mechanical strength and electrical performance when properly structured into fibrous assemblies. By uniting the intrinsic advantages of 2D nanosheets with the inherent toughness, conductivity, and weavability of fibers, this approach opens up promising pathways for creating high-performance wearable and flexible electronic devices.

Since its initial discovery by a research team at Drexel University in 2011, MXene materials have undergone just over a decade of development. Despite this relatively short history, the diversity in their chemical composition and structural forms has

enabled MXenes to exhibit a wide range of tunable electrical, magnetic, optical, thermal, and mechanical properties. In comparison with other two-dimensional materials, MXenes exhibit distinctive advantages, including metallic-like electrical conductivity, high volumetric capacity, as well as favorable biocompatibility—attributes not commonly found in graphene and related 2D systems. These advantages have positioned MXenes as promising candidates for a wide range of applications, including electromagnetic interference (EMI) shielding, electrochemical energy electrodes, sensing, and photoelectric conversion. For instance, Zhang et al. [6] fabricated a flexible film denoted as MXene/cellulose nanocrystal/acid-doped polyaniline using vacuum-assisted mixed filtration. Through careful interfacial engineering, the nanocomposite exhibited a 27% increase in shielding performance of shielding effectiveness (SE), attaining a maximum SE of 67.9 dB. In addition, the localized surface plasmon resonance effect of MXene contributed to improved energy conversion performance, suggesting a feasible strategy for designing integrated EMI shielding devices. In another study by Jiang et al. [7], a hybrid filler combining isocyanate-terminated polyurethane (PU) with hydroxyl-functionalized MXene nanosheets was introduced into an epoxy (EP) matrix, forming the MXene (0.1 wt%) /PU (1 wt%) / EP. This nanocomposite reached a peak EMI SE of 27.8 dB. The material also exhibited enhanced mechanical strength, electrical properties, and in situ damage detection capability, offering valuable insights for the development of multifunctional composite systems. A number of recent reviews have further elaborated on various facets of MXene-based composites—covering sensing, EMI shielding, flexible electronics, and wearable technology [8–10]. These analyses collectively underscore the significant potential of MXene nanosheets when integrated into multi-material composites, particularly in applications such as smart textiles, electromagnetic shielding, personal thermal management, sensing platforms, and advanced energy storage [11].

This chapter first explored the preparation methods and interfacial interactions of MXene fiber nanocomposite materials. Then, we introduced their related mechanical and electrochemical properties. Subsequently, this chapter was further extended to primary application areas to offer an overview of ongoing developments. Meanwhile, we discussed the current challenges and opportunities encountered, with the intention of making some contributions to the interdisciplinary field of materials science and technology through this chapter. We also intend to invest our own strength in the further development of MXene fiber nanocomposite materials.

2. Interface-engineered strategies

2.1 Interfacial interactions

Hydrogen bonding serves as a widespread mode of interfacial interaction in materials. MXene surfaces, rich in -O and -OH functional groups, can readily engage in hydrogen bonding with polar molecules such as water. For example, Jiang et al. [12] constructed an extensive hydrogen-bonded network within MXene layers using phytic acid (PA), in which phosphate groups ($\equiv\text{P}=\text{O}$) function as effective hydrogen bond acceptors. The incorporation of such organic molecules not only promotes hydrogen bond formation but also substantially strengthens the interlayer interface [13], resulting in improved mechanical properties and chemical stability of the material. Ionic bonding provides another strong interfacial mechanism [14], typically arising from electrostatic interactions between metal cations (e.g., Mg^{2+} and Ca^{2+}) and

anionic groups on MXene surfaces, such as -COO^- and -OH . Niu et al. [15] employed a hydrothermal approach to introduce Fe^{3+} and Mn^{2+} ions into MXene, significantly enhancing the overall material properties through this ion-mediated interfacial reinforcement. Covalent bonding offers a further route to enhance MXene interfacial strength, often formed between surface functional groups like -OH or -CHO and coupling agents such as N,N'-carbonyldiimidazole [16]. In one study, Zhou et al. [17] applied (3-aminopropyl) triethoxysilane modification to generate Ti-O-Si covalent linkages, which resulted in a remarkable 130% increase in fracture toughness. A comprehensive understanding of these interaction mechanisms—hydrogen, ionic, and covalent bonding—enables the rational design of MXene interfaces. By strategically combining weak and strong interactions, synergistic effects can be realized [18], leading to substantial enhancements in the mechanical behavior of MXene-based materials.

In earlier research, various strategies have been established to incorporate synergistic interfacial interactions into MXene-based nanocomposites. For instance, one study employed sequential bridging of MXene nanosheets using hydrogen bonds derived from sodium alginate and ionic crosslinking via calcium ions, resulting in MXene films exhibiting a tensile strength of 436 MPa and a Young's modulus of 14.0 GPa [16]. Li et al. [19] adopted a layer-by-layer blading coating technique to assemble MXene nanosheets with liquid metal and bacterial cellulose. This process improved nanosheet alignment and introduced multiple interfacial forces—including hydrogen bonds and $\text{C-O} \rightarrow \text{Ga}^{3+}$ coordination bonds—resulting in LBM films with a tensile strength as high as 908 MPa. During fiber fabrication, techniques such as thermal drawing, wet spinning, and coating have been utilized to integrate polymers and functional additives into MXene fibers, introducing hydrogen, ionic (e.g., Ca^{2+} , NH_4^+ , and Zn^{2+}), and covalent bonds to strengthen interfacial adhesion. Pure MXene fibers typically exhibit limited mechanical strength, often below 100 MPa. To address this, Cao et al. [20] incorporated hydrogen bonding during wet spinning, which reduced electrostatic repulsion and enhanced interfacial cohesion, leading to fibers with a strength of 157 MPa. Similarly, Liu et al. [21] fabricated core-shell structured composite fibers via wet coaxial spinning with MXene nanosheets, in which MXene nanosheets served as the core, surrounded by a shell of aramid nanofibers (ANFs). Leveraging hydrogen and ammonium ion bonding, the researchers achieved an ultra-high tensile strength (502.9 MPa) with a toughness of 48.1 MJ/m^3 . These studies highlight that the deliberate incorporation of multiple interfacial interactions (such as hydrogen, ionic, and covalent bonding) substantially enhances the mechanical properties of MXene-based composites.

2.2 Densification and induced orientation

Two key structural factors play a major role in determining the mechanical strength of MXene-based composite fibers: reduced porosity and improved nanosheet orientation. A high degree of alignment in the nanosheets significantly enhances load transfer and structural integrity within the composite [22]. Processes such as thermal drawing and tailored interfacial design help achieve tighter fiber packing and better-oriented MXene nanosheets, leading to notable gains in mechanical performance. For example, Gu et al. [23, 24] developed a structural design in which MXene nanosheets form an interpenetrating network with sliding-ring polyrotaxanes, effectively mitigating stress concentration. This configuration yielded fibers with a tensile strength reaching 502.3 MPa along with a toughness of 59.7 MJ/m^3 , while retaining

structural coherence even under significant strain. Similarly, in fluid-guided thermal drawing processes, MXene core-shell fibers can attain highly aligned architectures with minimal porosity, aided by interfacial synergy and thermally induced stress. An in situ-formed cyclic olefin copolymer (COC) protective layer further promotes the development of an interlocking sheet topology between the MXene core and the shell. This leads to an ultra-high tensile strength—reaching 707.7 MPa—as polymer chains and MXene nanosheets align under thermo-mechanical stress. With optimized drawing conditions, such fibers achieve an orientation parameter of 0.9 and porosity as low as 4.9% [25].

3. Preparation methods

MXene nanosheets possess abundant surface hydrophilic groups (e.g., -O and -OH), which facilitate stable dispersion in polar solvents and offer favorable processability. These characteristics allow MXene to be used directly as a spinning dope or integrated as functional fillers into fiber architectures, which can then be woven for use in functional wearable electronics. A range of fabrication techniques—including wet spinning, electrospinning, coating, biscrolling, and thermal drawing—has recently been developed to fabricate MXene fiber nanocomposites. Each method distinctly shapes the fiber's microstructure, which in turn governs its final functional and mechanical properties.

3.1 Wet spinning

MXene inks can form an ordered liquid-crystalline arrangement, making them suitable for fiber production through wet spinning [26]. In this method, nanomaterials are first dispersed into a spin dope, which is then extruded into a coagulating medium where solvent exchange occurs, leading to the formation of gel-state fibers [2]. Following stretching, drying, and winding, continuous filaments are obtained. Fibers' final properties are collectively influenced by processing parameters such as dope concentration, spinneret geometry, coagulation bath composition, and extrusion rate. Wet spinning is a widely adopted method in both industrial and textile applications and continues to serve as a classical spinning technique [27].

The fabrication of pure MXene fibers is still difficult, as the small size of MXene nanosheets and weak interlayer interactions limit their assembly at the macroscopic scale [26]. Adjusting the coagulation bath composition offers a promising strategy to address this issue. For instance, Eom's group [2] prepared continuous pure MXene fibers through wet spinning with an $\text{NH}_4\text{Cl}/\text{NH}_4\text{OH}$ coagulation system, achieving a high electrical conductivity (7713 S/cm) (**Figure 1**). It was found that NH_4^+ ions triggered gelation of the MXene dispersion, significantly improving spinnability; in the absence of such ions, continuous fibers could not be formed. In a similar approach, Cao et al. [20] produced Zn^{2+} -crosslinked MXene fibers using a coagulant containing ZnSO_4 and CaCl_2 in an ethanol/water mixture, achieving a tensile strength of 150.7 MPa, including electrical conductivity of 3637.9 S/cm. The improvement is attributed to Zn^{2+} ions, which mitigate electrostatic repulsion among adjacent MXene nanosheets, promoting tightly packed, ordered arrangements. Li et al. [28] further enhanced fiber microstructure by incorporating MgSO_4 into a conventional ethanol-water coagulation bath and optimizing the spinneret design, which effectively reduced structural defects such as pores and voids.

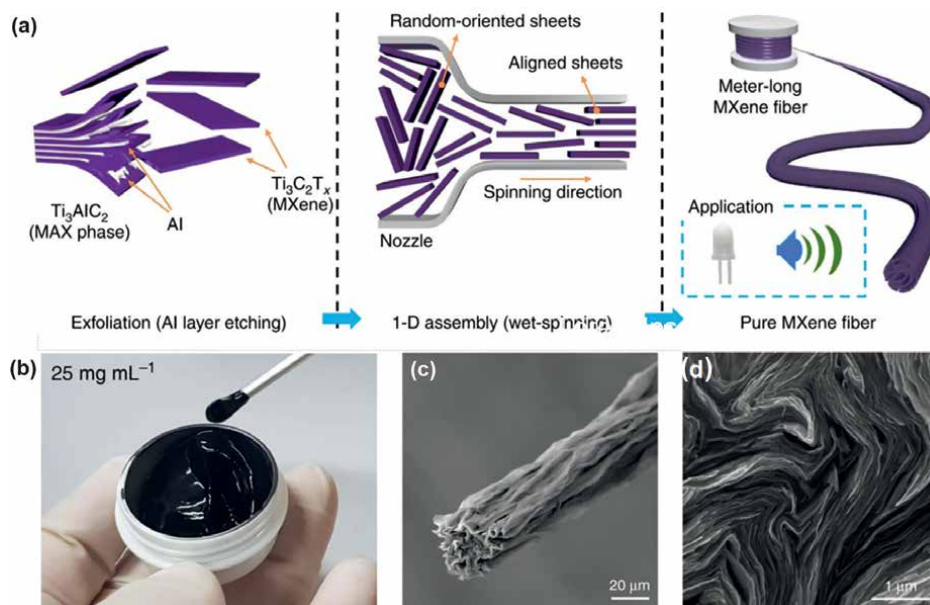


Figure 1. (a) Schematic representation showing the transformation of MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) single layers into MXene fibers. (b) Optical image of the concentrated MXene liquid-crystal dispersion with a concentration of 25 mg/mL. SEM images of fibers: (c) overall and (d) in cross-section [2].

To address the challenges of high spinning dope concentration and limited mechanical strength in pure MXene fibers, the fabrication of MXene-based composite fibers has emerged as a promising approach for addressing this challenge by researchers. The addition of polymers or other nanomaterials not only improves the spinnability of MXene dispersions at reduced concentrations but also increases the MXene loading within the fiber structure. Representative examples include MXene/polyrotaxane fibers [23], MXene/graphene oxide (GO) fibers [29], MXene/carbon nanotube (CNT) fibers [30], and MXene/cellulose nanofiber (CNF) fibers [31], among others. Gu et al. [23] prepared multifunctional nanocomposite fibers of high performance by integrating MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) nanosheets with a slide-ring polyrotaxane crosslinker—a mechanically interlocked polymer system composed of polyethylene glycol threaded through α -cyclodextrin rings. The approach yielded a reinforced internal structure, imparting excellent mechanical strength and electrical conductivity to the fiber. In another study, Yang et al. [29] reported a wet-spinning approach using GO liquid crystals as an aligning template for MXene nanosheets. This strategy enabled the continuous production of hybrid fibers containing up to 95 wt% MXene, where MXene sheets were uniformly oriented within the GO framework. Furthermore, wet spinning allows for the fabrication of multi-layered fiber architectures via coaxial spinning. Liu et al. [21] produced core-shell fibers featuring a conductive MXene core enveloped by a tough ANF shell. These fibers exhibited high tensile strength (502.9 MPa), including high electrical conductivity ($3.0 \times 10^5 \text{ S/m}$) and ultra-high toughness (48.1 MJ/m^3). The ANF shell also provided exceptional resistance to dynamic deformation, chemicals, extreme temperatures, and fire.

The shear forces generated during wet spinning induce alignment of MXene nanosheets, resulting in a high degree of orientation along the fiber axis [2]. Owing to

its operational simplicity, efficiency, and scalability, wet spinning is now among the most commonly employed methods for preparing MXene fiber composites [32].

3.2 Electrospinning

Electrospinning represents another extensively investigated approach for fabricating nanofibers, utilizing high-voltage electrostatic fields to draw fibers from polymer solutions, blends, or melts [33]. This technique is recognized for its operational simplicity, cost-effectiveness, and adjustable processing parameters [34]. The resulting electrospun mats possess a high specific surface area, structural flexibility, and tunable porosity, rendering them attractive for diverse functional applications [34].

During electrospinning, fiber formation is driven by electrostatic forces that elongate the polymer solution into thin filaments. In a conventional setup, a conductive polymer fluid is extruded through a syringe needle under high voltage, with the resulting fibers deposited onto a grounded collector such as a rotating drum or flat plate. MXenes, being readily dispersible in polar solvents like water and DMF, are particularly well-suited for integration into electrospun systems. For instance, Zhang et al. [35] developed an environmentally friendly, multifunctional Janus textile via sequential electrospinning (**Figure 2**). This asymmetrically layered structure combines an MXene-based radiative heating layer with a cellulose acetate (CA) cooling layer, allowing bidirectional thermal regulation under varying ambient conditions to achieve personalized thermal comfort.

The surface properties and functional group composition of MXene fibers create a conducive microenvironment for cellular adhesion and proliferation. Leveraging electrospinning and strategic doping, Huang et al. [36] developed intelligent MXene-based fibrous biomaterials suitable for cell culture and tissue engineering applications. The incorporation of abundant hydrophilic moieties significantly enhanced the wettability of the nanofibers. Biocompatibility assessments further confirmed positive cellular interactions and a substantial increase in cellular viability.

3.3 Coating

Coating provides a simple and equipment-friendly approach to depositing functional composite layers onto fiber substrates [37]. The process begins with the formulation of a homogeneous MXene dispersion, which is subsequently applied to pre-existing

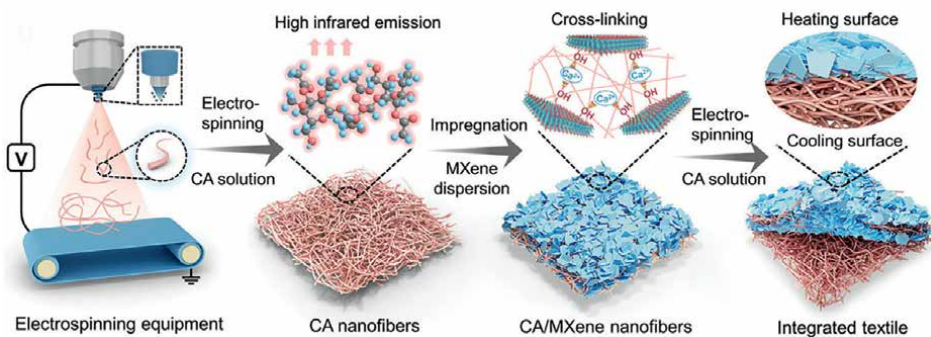


Figure 2.
Illustrated depiction of the procedure for fabricating the i-textile [35].

textiles, fibers, or yarns through techniques such as immersion [38] or spray deposition [39]. After application, the coated materials are air-dried at ambient temperature. Iterative coating cycles can be performed to enhance the total MXene content.

MXene surfaces are decorated with functional groups such as $-F$, $-O$, and $-OH$, conferring a net negative surface charge. This characteristic promotes electrostatic attraction and hydrogen bonding with positively charged, hydrophilic fiber matrices. In one demonstration, Lingyi et al. [40] established a scalable and continuous process for uniformly coating commercial nylon filaments with MXene at high speed (**Figure 3**). By exploiting the intrinsic electrical conductivity and process adaptability of MXene, the resulting fibers exhibited linear resistance values below $10 \Omega/\text{cm}$. These high-performance microelectrodes possess adjustable geometries and are applicable to various bioelectronic tasks, such as physiological monitoring and stimulation, providing new opportunities to investigate health- and disease-related mechanisms.

Despite its advantages in speed and scalability, the coating technique is constrained by limited MXene loading capacity and poor adhesion strength, often leading to coating detachment. These drawbacks ultimately compromise the functional and mechanical reliability of the composite fibers.

Although coating enables rapid, large-scale fabrication of MXene fibers composite, its effectiveness is hampered by difficulties in achieving high MXene loading and robust interfacial bonding, leading to compromised functional and mechanical performance [37].

3.4 Thermal drawing

Thermal drawing of fibers is a manufacturing process in which a macroscopic fiber preform is heated and stretched under tension to form thin, continuous filaments. This multi-step procedure involves preform fabrication, heating, drawing, cooling, and collection. The preform acts as a structural template whose dimensions

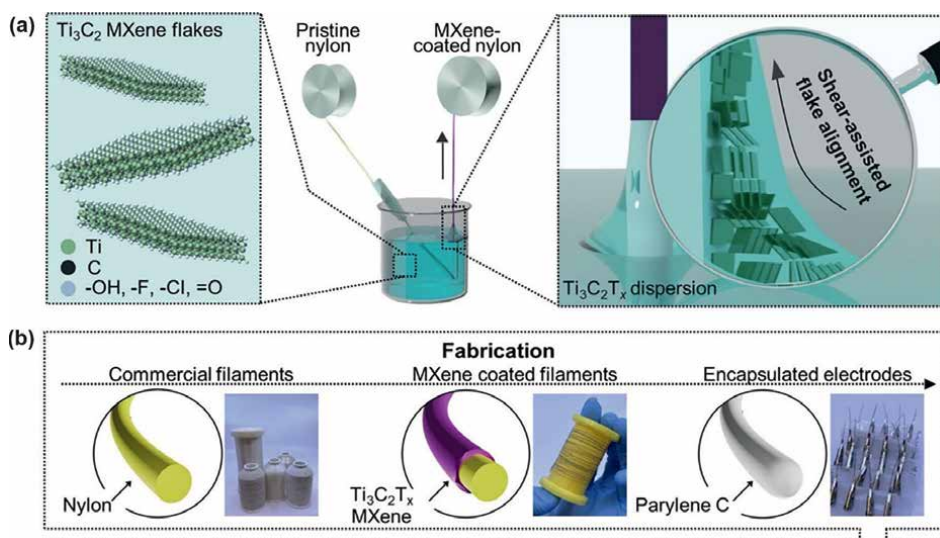


Figure 3. (a) Illustration of the dip-coating procedure, showing a nylon filament passing through a dispersion of MXene monolayers, where shear forces in the meniscus induce axial alignment of the flakes. (b) Corresponding schematics and images of bare nylon, MXene-coated, and Parylene-coated electrodes [40].

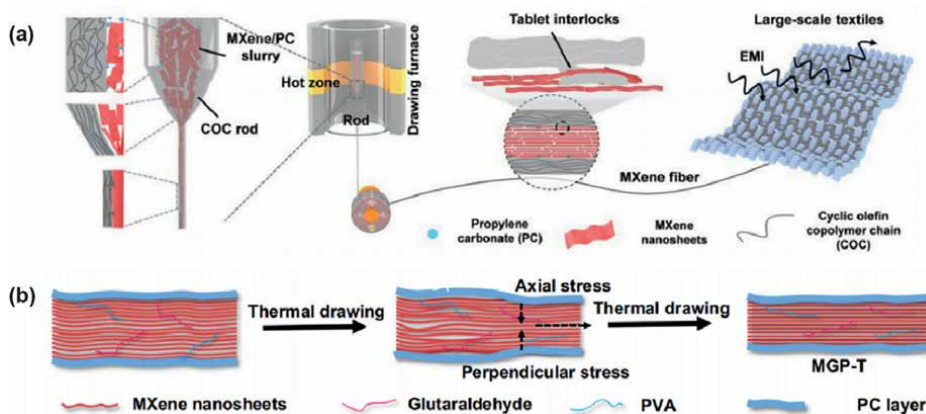


Figure 4. (a) Schematic illustration of the preparation route for MXene fiber nanocomposites, where a protective polymer layer is generated via direct thermal drawing [41]. (b) Diagram showing the formation mechanism of MGP-T fibers from MGP fibers under the combined action of axial and transverse stresses during thermal drawing [25].

and material composition critically influence the properties of the final fiber. When heated to a specific temperature, the glass or polymer component of the preform softens to a state suitable for stretching. Under controlled tension, the softened end is drawn downward at a constant rate, progressively reducing its diameter to the micrometer scale. Following elongation, the fiber is rapidly cooled to solidify its structure and retain the desired mechanical and functional characteristics.

In a representative study, Zhou et al. [41] established a continuous, controllable process to fabricate ultra-dense MXene fibers exhibiting high mechanical strength, toughness, as well as electrical conductivity (**Figure 4**). Initially, MXene nanosheets were employed to assemble into fibers via wet spinning, with polyvinyl alcohol (PVA) and glutaraldehyde (GA) serving as cross-linkers. The precursor fibers were subsequently inserted into a polymer hollow tube and thermally drawn. Tensile stress during drawing, together with the protective polymer layer formed in situ, facilitated dense packing of MXene nanosheets, producing fibers with improved structural integrity and performance.

By employing a fluidics-assisted thermal drawing technique, Zhou et al. [25] successfully fabricated kilometer-long MXene-based fiber composite with exceptional mechanical robustness, including high electrical conductivity. **Figure 4** illustrated that the fibers were formed by thermally co-drawing a MXene-dispersion core within a protective cyclic olefin copolymer (COC) cladding, which yielded an ultra-dense and highly aligned final structure.

4. Properties

MXene stands out by integrating remarkable mechanical strength, exceptional electrical conductivity, and efficient photothermal conversion capabilities, transcending the conventional trade-off of “single excellence” often seen in traditional two-dimensional materials. Furthermore, the surface chemistry of MXene is highly tunable, featuring an array of functional groups including -F, -O, and -OH. This chemical versatility enables the precise introduction of hydrogen, ionic, covalent, or

synergistic interfacial bonds, which collectively enhance material performance and broaden application potential. Complemented by its favorable biocompatibility and electrochemical properties, MXene holds significant promise across three strategic domains: energy, biomedicine, and environmental technology.

4.1 Mechanical property

Single-layer MXene nanosheets exhibit exceptional intrinsic mechanical characteristics. For instance, Lipatov et al. [42] performed nanoindentation tests on monolayer $\text{Ti}_3\text{C}_2\text{T}_x$ using atomic force microscopy, obtaining a tensile strength of 173 GPa along with an elastic modulus of 330 GPa. In a subsequent study, Rong et al. [43] refined sample fabrication and transfer techniques, directly facilitating in situ tensile evaluation of MXene sheets through a nanomechanical push-pull system. Their measurements revealed a tensile strength of 15.4 GPa along with a Young's modulus of 484 GPa. However, when MXene nanosheets are assembled into nanocomposite structures, their mechanical performance is often compromised by the emergence of pores and structural defects. Such defects commonly originate from poor interfacial wettability between polymer matrices and MXene as well as solvent evaporation during processing. Voids and imperfect contacts significantly undermine the structural integrity of composite materials. In addition, although MXene surfaces contain numerous functional groups (-F, -O, and -OH), the resulting interfacial bonding is often insufficient to achieve optimal load transfer [44]. As a consequence, the overall mechanical strength of MXene composites remains significantly lower than that of single MXene nanosheets. To address these limitations, recent research has focused on improving the structural integrity of MXene composites by minimizing porosity and enhancing nanosheet alignment [23, 25, 41, 45]. Equally important are strategies that strengthen interfacial crosslinking through hydrogen, ionic, or covalent bonding [45]. As elaborated in the previous section on synergistic interfacial interactions, these mechanisms offer efficient routes to translate nanoscale properties into improved macroscopic performance.

4.2 Electrical property

$\text{Ti}_3\text{C}_2\text{T}_x$ MXene demonstrates inherent electrical conduction superior to 10^4 S/cm and shows typical metallic temperature dependence, where its conductivity declines with increasing temperature. Experimentally, individual $\text{Ti}_3\text{C}_2\text{T}_x$ flakes have been measured to achieve conductivities as high as 2×10^4 S/cm [12]. Such outstanding conductive properties facilitate rapid electron transport through the material, which is essential for achieving millisecond-level sensor responses and the rapid charging/discharging performance needed in advanced energy storage systems [46]. In the fabrication of macroscopic MXene fibers, minimizing structural defects and improving nanosheet alignment help reduce interflake electron scattering, allowing the intrinsic conductivity of MXene to be more effectively utilized. As a result, fibers with higher orientation and fewer defects exhibit significantly improved electrical characteristics. Fabrication techniques, including wet spinning and post-drawing treatments, contribute to retaining high conductivity in the final fiber structures [2]. Further enhancements can be achieved by modulating surface functionalization and optimizing the in-plane orientation of nanosheets within the fiber architecture [47]. For example, Zhang et al. produced fibers via wet spinning using a chitosan-containing coagulation bath, attaining a notable electrical conductivity of 7748 S/cm [20].

MXene fibers show considerable potential for electromagnetic interference (EMI) shielding in next-generation smart electronics, owing to their high electrical conductance, hydrophilic nature, and tunable surface chemistry [48]. For instance, composite fibers manufactured via fluid-guided thermal drawing have been reported to exhibit exceptional electrical performance, with conductivities reaching 11959.4 S/cm [25]. When woven into textile form, these fibers deliver an EMI SE as high as 82 dB. Such high SE values not only reflect superior signal blocking capability but also come with notable stability and durability, positioning these textiles as promising candidates for high-performance electronic shielding applications.

4.3 Electrochemical property

The development of efficient energy storage technologies is vital to ensure the stable and effective deployment of clean energy sources. Electrode materials, serving as a core element in these systems, critically determine their overall electrochemical performance [49]. MXene has emerged as a highly promising intercalation-type electrode candidate due to its adjustable interlayer spacing, versatile surface chemistry, and outstanding electrical conductivity. First-principle calculations indicate that the hydrogen storage performance of MXenes depends on surface terminations, interlayer spacing, and the specific transition metals involved [50, 51]. In one investigation, Chu et al. [50] systematically compared the hydrogen adsorption behavior of MXenes with mixed surface functional groups against those with uniform terminations. Their results demonstrate that heterogeneous surface groups induce local dipole moments that strengthen hydrogen adsorption, reflected in higher average adsorption energies relative to uniformly functionalized systems. In a separate theoretical study, Cao et al. [52] employed density functional theory (DFT) to explore MXene structures with engineered local atomic environments. By designing carbon sites adjacent to nanopores, they successfully activated otherwise inert surface regions, achieving a theoretical potassium storage capacity that surpasses previously reported values for MXene materials.

4.4 Optical and thermal properties

Two-dimensional nanomaterials are known for their distinctive nonlinear optical behavior, and MXene—as an emerging member of this family—displays similarly remarkable optical performance [53]. For instance, titanium carbide ($\text{Ti}_3\text{C}_2\text{T}_x$) MXene shows strong saturable absorption across the 800–1800 nm wavelength range, with a maximum effective nonlinear absorption coefficient (β_{eff}) near $10^{-21} \text{ m}^2/\text{V}^2$. This value rivals or even exceeds that of many established two-dimensional materials [54]. Additionally, the surface chemistry of MXene with terminations like $-\text{O}$, $-\text{OH}$, and $-\text{F}$, is able to be dynamically reconfigured through electrochemical approaches [55]. This enables real-time modulation of its nonlinear optical response—a feature rarely attainable with conventional 2D counterparts.

In terms of thermal properties, MXenes like $\text{Ti}_3\text{C}_2\text{T}_x$ possess an in-plane thermal conductivity ranging from 50 to $100 \text{ W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$, outperforming most polymer-based systems. This advantage arises from their highly crystalline architecture and strong in-plane covalent bonds [56]. At the same time, MXenes exhibit outstanding photothermal conversion efficiency, with optical absorption exceeding 95% and photothermal conversion rates above 90%, positioning them as attractive candidates for integration into wearable thermal management devices [57].

4.5 Biocompatibility

Beyond its remarkable mechanical strength, electrical conductivity, and photo-thermal performance, MXene also exhibits excellent biocompatibility [58, 59]. Its high specific surface area and tunable terminations, along with inherent antibacterial activity further enable its use as a versatile drug carrier [60]. By conjugating with therapeutic agents and targeting ligands, MXene can facilitate precision drug delivery for targeted treatment. In addition, the material demonstrates favorable osteogenic properties and low biotoxicity, highlighting its potential for artificial muscle applications [61].

5. Application

5.1 Sensors

MXene fibers, leveraging their outstanding mechanical strength and electrical conductivity, are increasingly studied as sensing elements for integration into flexible and wearable electronic systems [9, 32, 46, 62, 63]. These fiber-based sensors are primarily categorized into two forms: strain sensors [8, 62] and pressure sensors [10, 63]. Both types function on a similar working mechanism—external mechanical stimuli such as stretching or compression from body movements cause structural deformation in the conductive MXene network, thereby modulating its electrical resistance [63]. The key distinction between them lies in the specific physical parameter detected and the directional nature of the resulting electrical signal variation.

5.1.1 Strain sensors

Strain sensors are used to detect mechanical deformation from body movements and translate it into measurable electrical signals. A common structural design involves embedding conductive MXene nanosheets uniformly within an elastic polymer matrix to establish a percolation network. Under applied strain, microcracks initiate and propagate, disrupting the conductive pathways and leading to a sharp increase in electrical resistance. For instance, MXene/polyurethane (PU) composite fibers fabricated by wet-spinning combine high MXene nanosheets' electrical conductivity with PU's stretchability, achieving a sensing range up to 152% and a gauge factor of $\sim 12,900$ [62]. The sensing mechanism of these composite fibers primarily relies on changes within the MXene conductive network during stretching. Deformation disrupts the electrical pathways, increasing resistance and enabling strain detection. To improve performance, fibers with MXene/PU as a sheath along with PU as a core were fabricated via a coaxial wet-spinning procedure, exhibiting improved cyclic stability. When knitted into textiles using industrial equipment, the resulting fabric could detect strains as high as 200% with a gauge factor around ~ 7.5 . Furthermore, a knitted elbow sleeve was developed based on this material, which successfully monitored various elbow movements by wirelessly transmitting signals via Bluetooth to a personal computer (**Figure 5**).

Another type of strain-sensing fiber utilizes aligned MXene nanosheets and operates on an inverse sensing mechanism. When stretched, the MXene lamellae slide and reorganize into a larger number of shorter conductive pathways, resulting in decreased electrical resistance. Through an interfacial crosslinking approach,

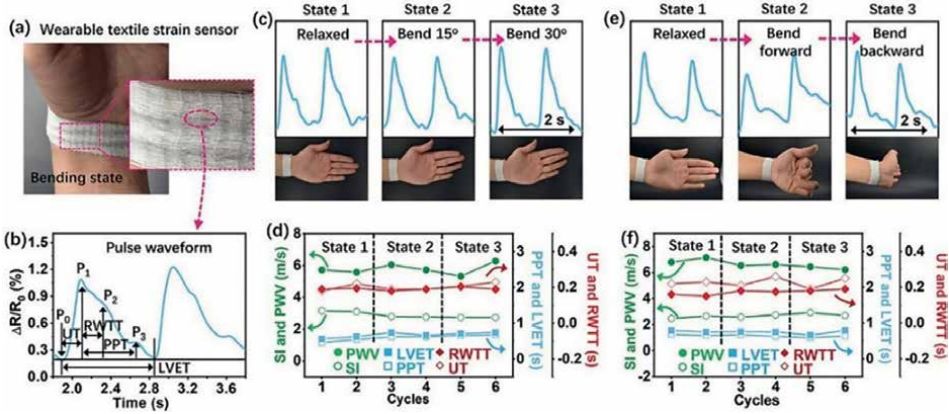


Figure 5. (a) Images of a wrist-worn cMP-fiber textile sensor for monitoring arterial pulse during wrist flexion. (b) Typical contour of arterial pulse signals obtained from the sensor. (c–f) Arterial pulse responses recorded by the sensor during various wrist motions [23].

researchers incorporated polyrotaxanes and Mg^{2+} ions into MXene fibers during wet spinning, producing a strain-sensing fiber with a sliding-enabled conductive network [16]. The resulting cMP fiber exhibits a unique response where stretching induces nanosheet alignment and formation of additional conductive connections, reducing resistance—contrasting with conventional fibers whose resistance increases under tension. Owing to its interlocked architecture, the cMP fiber maintains stable electrical responses under various mechanical disturbances such as stretching and bending, demonstrating strong interference immunity. This enables reliable monitoring of physiological signals—including pulse, facial expressions, and vocal vibrations—even during body movement. Integrated into wearable tactile sensors and attached to the skin, the fiber allows precise acquisition of pulse waveforms. In practical trials, the cMP sensor consistently captured pulse signals across different wrist motion states. Extracted clinical metrics—including systolic rise time, reflected wave transit time, and left ventricular ejection time—aligned well with established healthy baselines, confirming the sensor’s high stability and motion artifact resistance.

5.1.2 Pressure sensors

Pressure sensors represent another key class of sensing devices based on MXene fibers, functioning to convert external compressive forces into real-time electrical readouts. In contrast to strain sensors that can function with a single fiber, pressure detection typically relies on a crossed-fiber configuration. The fiber surfaces are intentionally designed to be microscopically rough and loosely packed; under applied load, the contact area at the junction expands significantly, leading to a measurable drop in contact resistance. As illustrated in **Figure 6**, a high-performance pressure sensor was constructed from MXene nanocomposite fibers through a two-stage fabrication route. First, MXene/carbon nanotube/polyurethane (MCP) composite fibers were wet-spun and then overcoated with MXene to trigger the in situ formation of cobblestone-inspired gold nanostructures (AuCNS), yielding AuCNS@MCP fibers [64]. The MCP fiber itself showed a sensitivity of 0.41 kPa^{-1} and an 83 ms response time, operating on the principle that applied pressure brings fibers into closer contact,

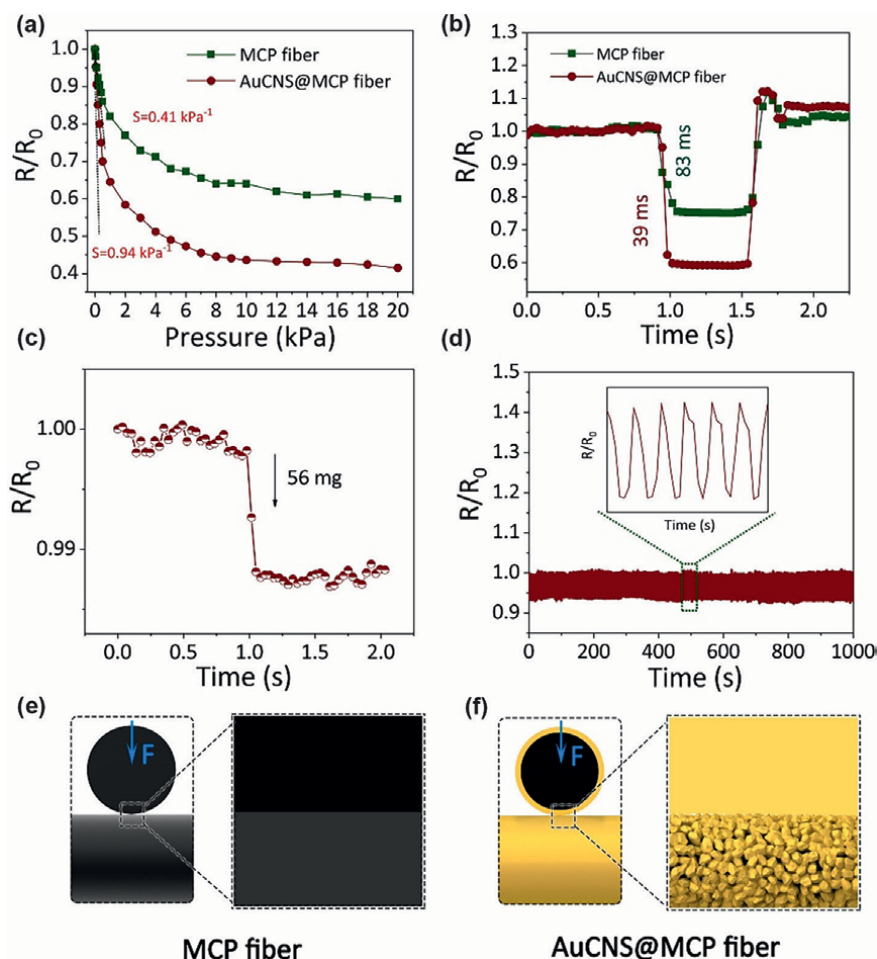


Figure 6.
 (a) Relative resistance of two perpendicularly stacked fibers under various pressures. (b) Response and recovery behavior of MCP and AuCNS@MCP-based sensors. (c) Sensitivity of the AuCNS@MCP sensor to a tiny force of 56 mg. (d) Cycling stability of the AuCNS@MCP sensor during repeated loading/unloading. Schematic diagrams illustrating the sensing mechanism of (e) MCP fibers and (f) AuCNS@MCP fibers [64].

boosting conductive pathways and lowering resistance. The AuCNS-modified fiber, with its nano-structured gold coating, further amplifies this effect by increasing the number of contact points and effective surface area, resulting in greater resistance variation and enhanced performance—achieving 0.94 kPa^{-1} sensitivity and a 39 ms response time. This sensor also detects subtle forces ($\sim 56 \text{ mg}$) and maintains consistent output over 1000 loading-unloading cycles, demonstrating high stability.

5.2 Supercapacitors

Supercapacitors are highly valued in the field of compact and flexible electronics because of their excellent specific capacitance, fast charge-discharge rates, and high durable cycling performance [65]. With increasing societal demand, the development of lightweight, portable, and high-performance wearable supercapacitors has gained significant attention. MXene fibers, characterized by their inherent metallic

conductivity, high volumetric capacitance, hydrophilicity, aqueous processability, as well as mechanical flexibility and durability, have emerged as promising materials for wearable energy storage electronics [66–68].

In one study, a simple coating process was used to deposit MXene directly onto silver-coated nylon fibers, producing an all-solid-state flexible supercapacitor. The resulting device delivered a high areal capacitance (328 mF/cm^2) along with remarkable cycling stability. Even under repeated bending, twisting, and knotting, the supercapacitor retained over 80% of its initial capacitance, demonstrating excellent mechanical ruggedness and adaptability [66]. These properties make such fiber-based supercapacitors a suitable energy supply component for integration into wearable electronics (**Figure 7**).

Employing a wet-spinning approach, MXene/graphene oxide (GO) hybrid fibers with a high MXene content of approximately 88 wt% were fabricated. In a 1 M H_2SO_4 electrolyte, these fibers delivered a volumetric capacitance as high as 341 F/cm , including an electrical conductivity of 72.3 S/cm^1 . The assembled supercapacitor achieved a maximum energy density of 5.1 mW h/cm^3 along with a peak power density of 1700 mW/cm^3 , while also maintaining stable charge-discharge performance over 20,000 cycles [67]. Beyond their electrochemical advantages, the fibers retained both flexibility and mechanical integrity, positioning them as a promising

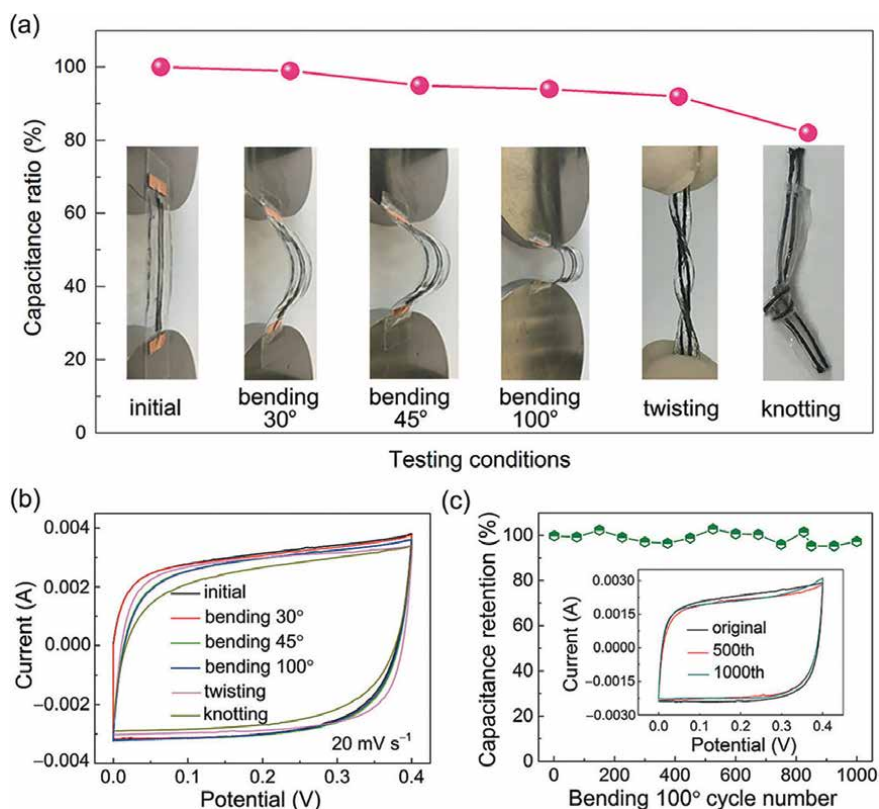


Figure 7. (a) Normalized capacitance (C/C_0) of the fiber supercapacitor under multiple deformation modes at 20 mV/s . (b) CV profiles under different test conditions at 20 mV s^{-1} . (c) Specific capacitance as a function of bending cycles at 100° ; the inset shows CV curves after 500 and 1000 cycles [66].

material for fiber-shaped energy storage components in wearable and miniaturized electronics. Using electrospinning, MXene flakes were combined with polyacrylonitrile (PAN) in a DMF solvent to form composite fibers incorporating up to 35 wt% MXene. Subsequent carbonization at 800°C yielded free-standing electrodes composed of MXene/carbon nanofibers. These electrodes achieved an area capacitance up to 244 mF/cm² in 1 M H₂SO₄ electrolyte, substantially surpassing the performance of pure carbon nanofiber counterparts. The introduction of MXene markedly improves the electrochemical behavior of the electrodes, rendering them highly suitable for wearable supercapacitors while also showing potential for applications in areas such as filtration and electrocatalysis.

5.3 Electromagnetic interference shielding

As intelligent and high-performance portable electronics become more prevalent, managing EMI has emerged as a critical concern. Such interference not only risks data corruption and operational failure of electronic equipment but may also present potential health hazards [68–71]. Moreover, the ongoing advancement of flexible and wearable electronics demands EMI shielding materials that are lightweight, thin, processable, and mechanically compliant, without compromising shielding effectiveness. MXene-based materials, with their metal-like electrical conductivity, mechanical robustness, and intrinsic flexibility, constitute a promising candidate for next-generation EMI shielding applications [51, 72, 73].

Feng et al. [74] engineered a coaxial fiber with a carbon nanotube (CNT) shell and an MXene core via wet spinning, as depicted in **Figure 8**. By carefully tuning the MXene-to-CNT ratio, they established a conductive gradient within the fiber, which promotes the emergence and subsequent absorption of electromagnetic waves. Fabrics woven from this fiber achieved an EMI SE of 23.40 dB within the X-band, with an absorption coefficient of 0.63. The protective CNT sheath ensured stable electrical performance even after bending, stretching, and ultrasonication, and the fabric maintained reliable EMI shielding in both open and enclosed spaces.

A continuous and well-controlled manufacturing strategy has been established to produce high-quality MXene fibers with protective layers formed in situ, leveraging the synergistic effects between interfacial interactions and drawing stresses [41]. As a result, the ultracompact fibers not only possess high tensile strength, remarkable toughness, and excellent electrical conductivity but also maintain a highly aligned structure with minimal porosity. Textiles woven from these MXene fiber composites demonstrate remarkable EMI shielding performance. When electromagnetic waves impinge on the fabric surface, the abundant free electrons in MXene rapidly respond, reflecting a portion of the incident energy. The residual waves penetrate the lattice of MXene, interacting strongly with its internal electrons. This interaction induces localized currents that effectively dissipate electromagnetic energy. Owing to the multi-layered architecture of MXene, incoming waves undergo repeated internal reflections between adjacent nanosheets, leading to progressive attenuation and eventual absorption.

5.4 Thermal management

For daily protection, flexible and wearable textiles are increasingly required for routine human thermal regulation. MXene fiber nanocomposites, which have high electrical conductivity, are renowned for their excellent thermal conductivity.

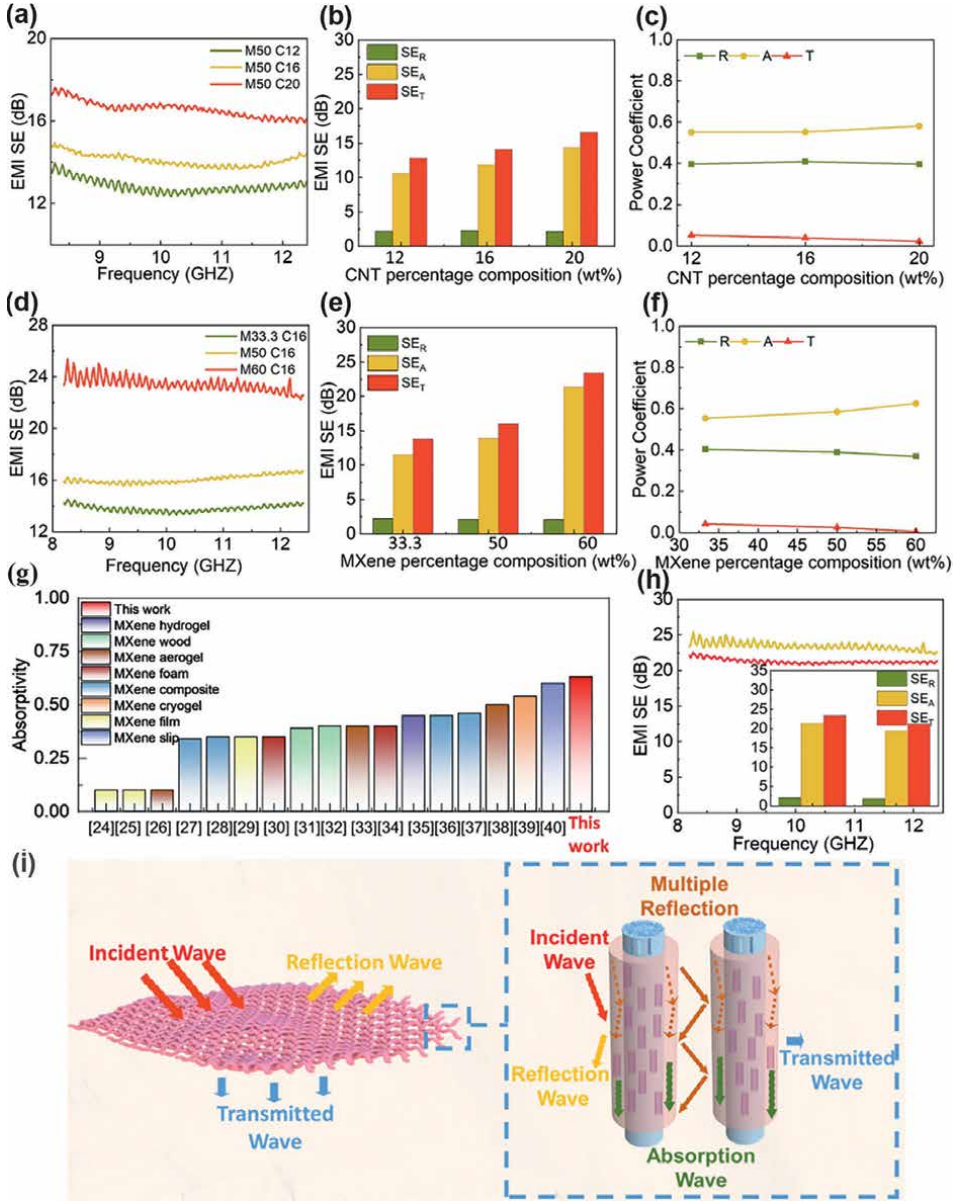


Figure 8. (a) EMI SE performance of CNT/MXene textiles. (b) Average SE_R , SE_A , and SE_T of CNT/MXene textiles in the X-band. (c) Absorption (A), transmission (T), and reflection (R) of CNT/MXene textiles in the X-band. (d) EMI SE images of CNT/MXene textiles. (e) Average SE_R , SE_B , and SE_A of CNT/MXene fabrics in the X-band. (f) A, R, and T of CNT/MXene textiles in the X-band. (g) Comparison of A values for different MXene-based materials reported in the literature. (h) EMI stability of CNT/MXene textiles under repeated testing. (i) Schematic diagram illustrating the electromagnetic shielding mechanism of CNT/MXene textiles [74].

Wang et al. [75] employed a point-sheet crosslinking strategy that enabled concurrent optimization of interlayer spacing and both intra- and interlamellar crosslinking within MXene fibers, yielding synergistic enhancements in electron and ion transport (**Figure 9**). The resulting fibers demonstrated outstanding electrical conductance (2405 S/cm), high volumetric capacitance (1597 F/cm³), and a remarkable energy

density (19.8 mWh/cm^3). Beyond their utility in assembling supercapacitors, the fibers also exhibited efficient joule heating and photothermal response. These multifunctional attributes make them suitable for practical applications such as powering LEDs and managing heat in portable electronics.

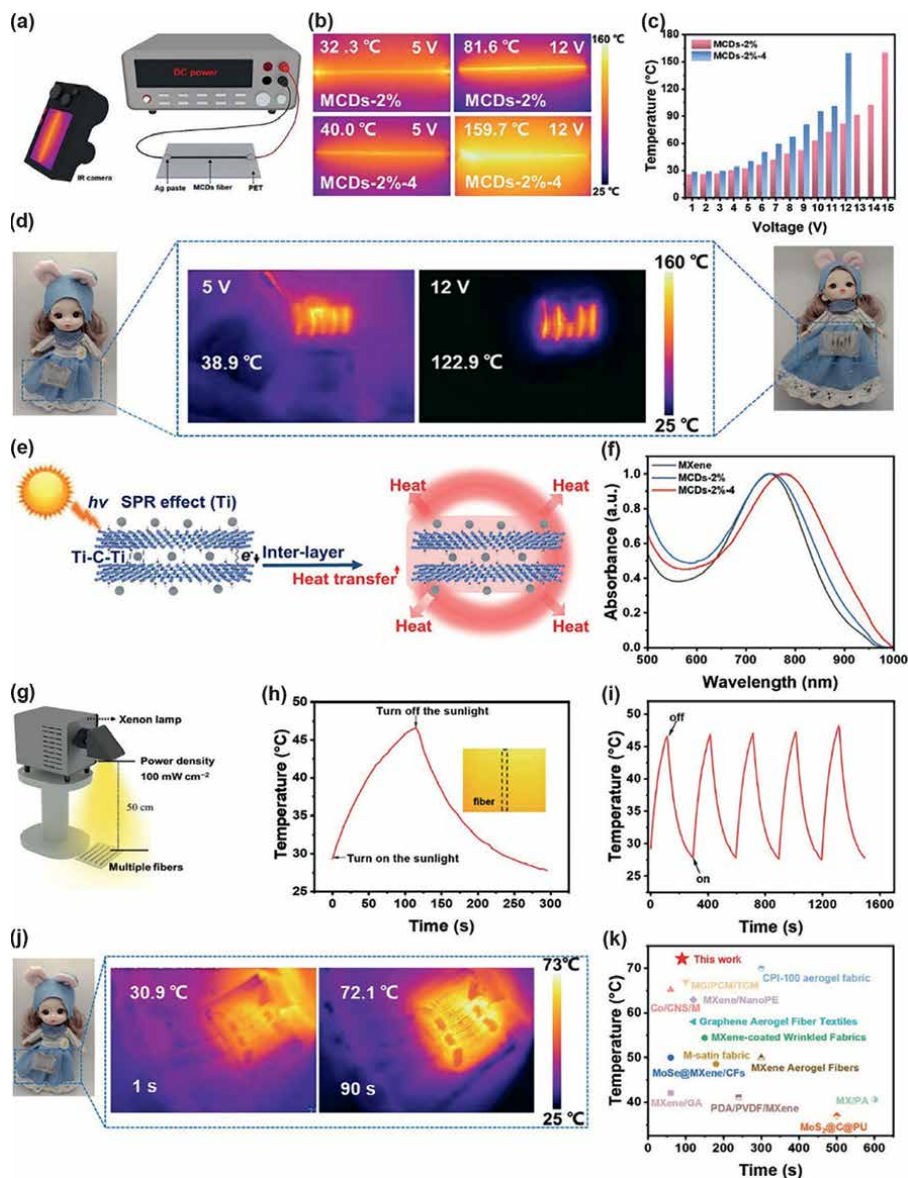


Figure 9. (a) The illustration of measuring the Joule heating effect of MXene-based fibers. (b) Infrared images, respectively, at 5 and 12 V and (c) voltage-dependent temperatures of MCDs-2% and MCDs-2% - 4 fibers. (d) Infrared images of MCDs-2% - 4 fiber-based fabric under the loaded voltages of 5 and 12 V, respectively. (e) Schematic illustration for the mechanism of photo-thermal energy conversion for MCDs-2% - 4 fibers. (f) UV-NIR absorbance spectra of MXene, MCDs-2% and MCDs-2% - 4. (g) Schematic diagram of simulated photo-thermal test (power density = 100 mW/cm^2). (h) Time-dependent temperature variations of a single MCDs-2% - 4 fiber under the sun. (i) Temperature variations of MCDs-2% - 4 fiber with light on/off for five cycles. (j) Infrared images of MCDs-2% - 4 fiber-based fabric under the sun. (k) Photo-thermal conversion performance of MCDs-2% - 4 fiber in comparison with the reported materials under the sun [75].

5.5 Optics

MXene fibers show considerable promise for photothermal applications due to their broad-spectrum light absorption—spanning ultraviolet to infrared—and their pronounced localized surface plasmon resonance. When irradiated, photons excite electrons in the material, which rapidly transfer energy to the lattice through strong electron–phonon interactions, resulting in efficient and rapid heat generation.

This photothermal effect can be strategically applied to improve the antibacterial performance of textile materials. In one example, Yan et al. [76] reported that silk fabrics coated with MXene and irradiated with sunlight achieved an *Escherichia coli* reduction rate exceeding 95%, compared to less than 20% under non-irradiated or uncoated conditions (Figure 10).

5.6 Biocompatibility

The development of flexible electronics and medical monitoring devices depends heavily on the performance of conductive fibers [77, 78]. Due to their high electrical conductance and flexibility, MXene fibers show considerable promise for such applications. For instance, Cheng et al. [79] integrated KM fibers (Kevlar/MXene

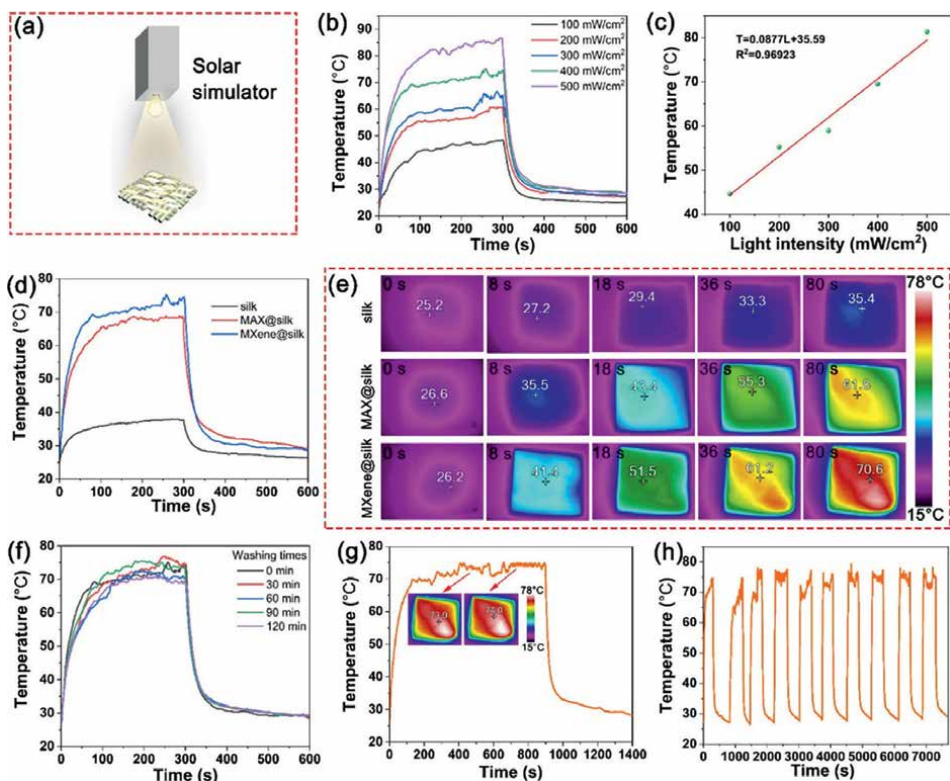


Figure 10.

(a) Schematic of samples under simulated sunlight irradiation. (b) Variation of surface temperature over irradiation time under different light intensities. (c) Linear correlation between light intensity and surface temperature. (d–e) Time-dependent temperature curves and IR images of different samples. (f) Influence of washing cycles on textiles photothermal behavior. (g) Long-term surface temperature changes under continuous irradiation (insets: IR images). (h) Cycling stability of the photothermal performance [76].

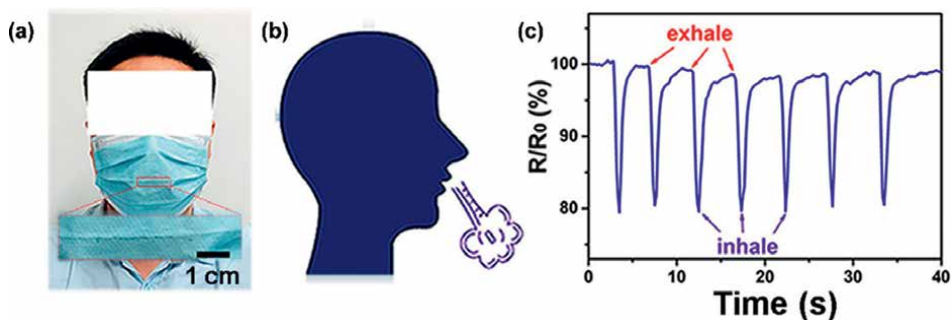


Figure 11. (a) Image showing breathing with a disposable medical sensory mask. (b) Diagrammatic representation of breathing. (c) Resistance versus time curve of the textile sensor during normal respiration [79].

hybrid fibers) onto conventional medical masks, creating a functional mask capable of monitoring human respiration, as shown in **Figure 11**. The sensing mechanism relies on the negative temperature coefficient (NTC) behavior of MXene, wherein the electrical resistance decreases as the temperature rises. When the wearer exhales warm air, the sensor on the mask surface undergoes a rapid resistance drop. During inhalation of cooler ambient air, the resistance recovers to its baseline level. This reversible and sensitive resistance variation allows real-time tracking of the wearer's breathing pattern.

6. Conclusion

This chapter examines the fabrication of MXene-based fibers, highlighting interfacial design strategies that improve mechanical strength and electrochemical behavior through tailored synthesis routes. Such progress supports interdisciplinary applications in sensing, energy storage, EMI shielding, personal thermal management, and related fields. With their optimized performance, these fiber materials can be effectively incorporated into flexible and wearable device platforms. Despite the rapid evolution of MXene composite fibers, several fundamental and technical challenges still require resolution. The main outstanding issues are summarized as follows:

1. The dimensions, structural integrity, and surface chemistry of MXene nanosheets strongly influence their liquid crystalline behavior, which in turn governs the properties of the assembled fibers. Increasing the lateral size of the nanosheets is highly desirable. At present, the limited production yield and stringent synthesis conditions of MXene nanosheets hinder the widespread adoption of MXene fibers. It is thus essential to develop more efficient and scalable synthesis routes to enhance nanosheet quality and processability.
2. The mechanical and electrical performance of macroscopic MXene fibers is still significantly inferior to that of single nanosheets. This discrepancy results from structural defects—such as wrinkles, misalignment, and voids—formed during fiber assembly. To address these issues, processing methods should be refined, for example, by applying higher shear forces during spinning and implementing post-drawing treatments, to improve nanosheet orientation and reduce internal porosity.

3. Insufficient interlayer bonding between MXene nanosheets restricts effective stress transfer, thereby limiting the strength, toughness, along with electrical conductivity of MXene fibers. Meanwhile, enhancing interfacial interactions—through crosslinking or functionalization—is critical to improving load and electron transfer across nanosheets and achieving better macroscopic performance.
4. The fabrication of MXene-based textiles remains largely confined to laboratory settings. To enable real-world application, scalable and continuous production methods must be established. Advancing high-throughput manufacturing technologies will be key to bridging the gap between lab-scale innovation and commercial deployment of high-performance MXene fibers.

With continued interdisciplinary efforts, further breakthroughs are expected to refine the performance and expand the application scope of these fibrous materials. The convergence of materials science, nanoscale engineering, and advanced manufacturing is establishing MXene fibers as a foundational component in the next generation of functional material systems.

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Conflict of interest

The authors declare no conflict of interest.

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MXenes for Wearable Multifunctional Sensing and Artificial Intelligence Devices

Long Chen

Abstract

The exponential growth of artificial intelligence (AI) has led to an escalating demand for energy-efficient, data-intensive computing solutions. Conventional von Neumann architectures, constrained by inherent memory-processor bottlenecks, struggle to meet these requirements. Neuromorphic devices enable energy-efficient, scalable, and high-speed neuromorphic computing, potentially addressing the von Neumann bottleneck and the limits of Moore's Law. Two-dimensional MXene materials, with their excellent mechanical and electrical properties, have become a transformative platform for developing neuromorphic devices, providing unparalleled advantages in sensing, nonvolatile memory, and bio-inspired computation. This chapter systematically summarizes recent advances in MXene-based flexible neuromorphic memristor devices. First, we delineate materials engineering strategies for synthesizing MXene thin films with tailored electronic and mechanical properties. Next, we classify MXene-derived neuromorphic materials and elucidate their switching mechanisms, including ion migration and charge trapping. A critical analysis of MXene-enabled devices highlights breakthroughs in-memory, artificial synapses, neuromorphic circuits, and multimodal in-sensor computing. Finally, we discuss persistent challenges in stability, scalability, and interfacial engineering, while projecting future directions for MXene-integrated sensing-memory-processing systems. This chapter provides a potential pathway for leveraging MXenes to transcend the limitations of conventional computing paradigms.

Keywords: emerging 2D materials, flexible electronics, neuromorphic, artificial intelligence, wearable applications

1. Introduction

The rapid progress of machine learning and artificial intelligence technologies has imposed revolutionary requirements on high-performance electronic devices [1]. To adapt to this technological evolution, academia is actively developing “edge computing,” which combines high transmission rates, large storage capacity, non-volatility, and low operating voltage [2–4]. While deep neural networks

demonstrate enormous potential in data storage and processing, their training processes, which involve optimizing tens of thousands of parameters, have exposed computational bottlenecks and memory wall limitations in traditional architectures. Notably, the human brain, as a naturally efficient computing system, achieves advanced functions such as cognitive decision-making and information storage through a complex network of approximately 10^{11} neurons and 10^{15} synapses, consuming merely 20–30 W of power [4]. Its storage density reaches 50,000 times the total text volume of the U.S. Library of Congress. In contrast, traditional computers not only exhibit significant performance gaps but also suffer from 100-watt-level energy consumption and the inherent von Neumann architecture limitations in-memory-computation separation, highlighting the constraints of existing technological approaches [4–7].

To transcend conventional computing paradigms, researchers have proposed neuromorphic computing concepts that implement memory-computation integration by mimicking the structures and functions of the biological brain. Carver Mead first introduced the concept of “neuromorphic engineering” in 1990, developing brain-inspired hardware [8]. Within this framework, artificial synapses not only serve as neural signal transmitters but also function as fundamental computational units. Memristors featuring programmable resistance characteristics have gotten significant attention because of their unique resistive switching (RS) effects: their resistance values undergo reversible changes under applied voltage modulation through thin-film sandwich structures. This resistance-switching mechanism originates from the dynamic conductive filaments (CFs) formation and rupture between electrodes, enabling devices to simulate synaptic plasticity and achieve deep integration of memory and computation [9]. Although metal-oxide memristors have been extensively studied, their spatiotemporal consistency defects have prompted the exploration of new 2D material systems [10]. Among these, MXene (transition metal carbide/nitride) has become a novel material platform for memristors and electronic synaptic devices, owing to its excellent conductivity, wide bandgap characteristics, and exceptional thermal stability [11].

Since the first report of $\text{Ti}_3\text{C}_2\text{T}_x$ in 2011, the MXene family has expanded to include numerous members through the regulation of transition metal elements and carbon/nitrogen ratios [12]. Their layered structure endows the material with a high specific surface area, tunable interlayer spacing, superior electrical/thermal conductivity, and surface functionalization potential—properties that align perfectly with neuromorphic device design requirements [13]. Compared to the stability deficiencies of organic-inorganic hybrid perovskites and the durability limitations of 2D materials like molybdenum disulfide and black phosphorus, MXene’s ability to maintain stable performance under harsh conditions highlights its advantages for flexible electronics and extreme-environment applications [14, 15]. Current research confirms that MXene-based memristors not only accurately simulate neural behaviors, including spike-timing-based plasticity (STDP) but also achieve breakthroughs in critical metrics, including data storage density and operating voltage. This chapter systematically reviews recent progress in MXene-based memristor design and neuromorphic computing, with particular emphasis on its application potential in artificial synapses and neuromorphic sensing computing, providing theoretical guidance and technical roadmap references for next-generation information technology device development.

2. Main text

2.1 Synthesis and preparation strategy for MXenes

The versatility of MXenes—two-dimensional transition metal carbides/nitrides—has driven their exploration in diverse material forms, including powders, hydrogels, and thin films. Despite advancements in MXene diversification, thin-film architectures remain dominant due to their compatibility with scalable manufacturing and multifunctional applications. MXene films exhibit exceptional promise as flexible electrodes, ion-selective membranes, battery separators, and molecular sieves, leveraging their crystallographic anisotropy, tunable surface chemistry, and mechanical robustness [13, 14]. MXene nanosheets self-assemble into freestanding films *via* van der Waals interactions, but excessive interflake forces cause restacking, reducing accessible active sites and surface area. Therefore, interlayer spacers—such as polymers, carbon nanomaterials (e.g., CNTs, graphene), and inorganic nanoparticles—are inserted between MXene sheets [13]. Furthermore, post-synthesis annealing optimizes surface terminations (e.g., reducing –F and –OH groups), enhancing electrochemical activity.

2.1.1 Vacuum-assisted filtration (VAF)

The synthesis of aligned MXene films involves a precisely controlled interfacial assembly process. First, an aqueous MXene dispersion is vacuum-filtered onto a porous substrate, where MXene nanosheets rapidly adsorb onto the membrane's pore surfaces. At the liquid-air interface, these nanosheets undergo face-to-face densification, forming a gel-like phase through hydrogen bonding and van der Waals interactions. Subsequent solvent evaporation generates capillary-induced compressive stresses perpendicular to the nanosheet planes, driving interlayer packing with sub-nanometer spacing. After drying, the freestanding MXene film is delaminated from the substrate, exhibiting anisotropic conductivity and mechanical strength [15]. This process exploits MXenes' hydrophilic terminal groups (–O, –OH) to form hydrogen-bonded interlayers, yielding membranes with characteristic wrinkled morphologies. For example, Ling et al. engineered conductive MXene/PDDA films through electrostatic interactions between negatively charged $\text{Ti}_3\text{C}_2\text{T}_x$ and cationic poly(diallyldimethylammonium chloride) (PDDA), achieving ordered layer stacking and mechanical flexibility [16]. In hydrophilic polymer blends, MXene/polyvinyl alcohol (PVA) composites (0.3 mg/mL MXene + 0.1 wt% PVA) demonstrated a volumetric capacitance of 530 F/cm³ and conductivity of 2.2×10^4 S/m, attributed to PVA's hydroxyl-mediated dispersion stabilization [17, 18]. Coating polyvinylidene fluoride (PVDF) substrates with $\text{Ti}_3\text{C}_2\text{T}_x$ reduced water contact angles from 81° (pristine PVDF) to 37°, improving filtration efficiency [19]. Although planar MXene architectures can be mechanically cut into diverse geometries, their assembly into complex multiscale 3D structures faces inherent limitations. Traditional adhesive-based bonding introduces foreign residues that compromise intrinsic conductivity and mechanical integrity. In contrast, welding—a process relying on atomic/molecular diffusion at interfaces—enables seamless integration of materials like metals or thermoplastics without additives [13]. Hydrated MXene doughs containing

interlamellar water molecules exhibit self-adhesive properties *via* reversible hydrogen bonding and van der Waals interactions. This raises a critical question: Can solid-state MXene laminates, retaining trace interfacial water from colloidal processing, undergo analogous “cold welding” under controlled stimuli? Through this welding strategy, high-quality MXene films show significant potential for various applications.

2.1.2 Spin-coating

Spin-coating is recognized as a highly efficient and rapid technique for fabricating uniform MXene-based films, offering significant advantages in material processing and device fabrication. The process typically involves preparing a homogeneous MXene colloidal solution through intense stirring or ultrasonication with additives, followed by precise deposition onto a clean substrate. Under controlled centrifugal force, temperature, and vacuum conditions, solvent evaporation forms high-quality composite films that can be easily detached for diverse applications [4]. The effectiveness of this technique has been demonstrated by fabricating transparent MXene contacts *via* spin-coating, which were integrated into Ti_3C_2 -based MXene photodetectors. This approach produced transparent MXene films that improved device performance, achieving a fourfold enhancement in photodetector sensitivity compared to conventional gold-based counterparts by optimizing carrier transmission distance and responsiveness. Similarly, highly transparent, conductive, and structurally ordered $\text{Ti}_3\text{C}_2\text{T}_x$ films were fabricated through spin-coating and implemented in transparent solid-state supercapacitors. Vacuum annealing at 200°C yielded continuous transparent films with large $\text{Ti}_3\text{C}_2\text{T}_x$ sheets aligned parallel to the substrate, exhibiting excellent electrical and optical properties [4, 13].

Dillon et al. advanced the field by producing ultrathin spin-coated $\text{Ti}_3\text{C}_2\text{T}_x$ films with thicknesses of ~ 50 nm and excellent conductivity [20]. This method surpassed the limitations of earlier MXene optical studies using physical vapor deposition, with high conductivity through spin-coating. Huang et al. developed a low-cost treat-cut-coat method for $\text{Ti}_3\text{C}_2\text{T}_x$ MXene film [21]. The resulting interdigitated MSCs achieved high areal and volumetric capacitances while maintaining excellent capacitance retention. This work represents a significant advancement in miniaturized energy storage technology.

2.1.3 Direct deposition

Physical vapor deposition (PVD) enables atomic-scale material construction, producing high-quality films [22]. However, high-temperature PVD $>700^\circ\text{C}$ poses challenges for temperature-sensitive materials. Chemical Vapor Deposition (CVD) synthesizes MXenes under thermodynamic equilibrium at high temperatures. Unlike PVD, which operates under kinetically controlled conditions, CVD allows limited control over lateral material growth. The first CVD synthesis of MXene films (Ti_3SiC_2) produced pure-phase Ti_3SiC_2 films at extremely high temperatures (1000 – 1300°C) and involved simultaneous deposition of all constituent elements alongside gas-solid reactions (e.g., TiC formation), a process known as reactive CVD [23]. To date, CVD has seen limited application in MXene synthesis beyond Ti_3SiC_2 , presenting an exciting avenue for future research.

2.2 Memristive switching mechanisms of synthesis and preparation strategy

The continuous advancement of MXene-based memristive materials necessitates a thorough understanding of their switching mechanisms to optimize device performance. Both theoretical calculations and experimental studies have identified two predominant mechanisms governing resistive switching behaviors: filamentary conduction and charge trapping.

2.2.1 Filamentary conduction

Filamentary conduction is a dominant switching mechanism in MXene-based memristors, heavily influenced by the choice of active materials and electrodes. This mechanism typically operates through two distinct conduction mechanisms of valence change memory (VCM) and electrochemical metallization memory (ECM) (**Figure 1a**). In ECM-based memristors, active metals such as silver (Ag) and inert metals like copper (Cu) are commonly used as electrodes [24]. The switching process begins when a positive voltage bias is applied to the top electrode, causing the active metal to oxidize at the anode. This oxidation generates metal cations, which migrate through the active layer under the influence of the applied electric field. Upon reaching the cathode, these cations are reduced to form neutral metal atoms, which accumulate and eventually form conductive filaments. Once these filaments bridge the two electrodes, the device transitions from a high-resistance state (HRS) to a low-resistance state (LRS), significantly enhancing conductivity. Conversely, when a reverse voltage bias is

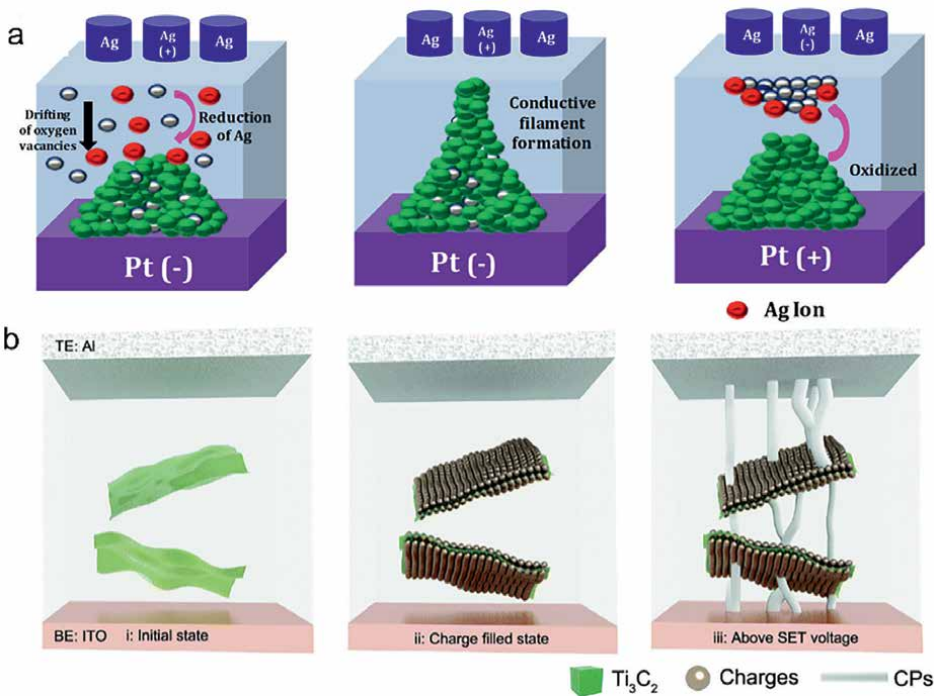


Figure 1.
Schematic of the mechanism [24]. (a) Filamentary conduction. (b) Charge trapping mechanism.

applied, the metal atoms at the base of the filament oxidize back into cations, leading to the dissolution of the filaments. This process reverts the device to its initial HRS, completing the reversible switching cycle. A notable example of ECM behavior was demonstrated by Khot et al. in an Ag/Ti₃C₂/Pt memristor [24]. In this device, the active Ag electrode facilitated the formation and rupture of conductive filaments within the Ti₃C₂ functional layer, driven by electrochemical redox reactions of Ag. This research highlighted the critical role of filamentary conduction in achieving reliable memristive switching.

Valence Change Memory (VCM)-based memristors rely on the migration of donor-type defects, such as atomic vacancies, within the active layer to form conductive filaments. A prominent example involves the migration of oxygen vacancies [25]. When an external voltage is applied, oxygen ions within the active layer migrate toward the anode, leaving behind a high concentration of oxygen vacancies. These vacancies aggregate near the cathode and diffuse into the active layer, forming oxygen-deficient conductive filaments that modulate the device's conductivity. Similar to ECM, VCM exhibits reversible bipolar switching under opposing electric fields. Khot et al. also fabricated a Pt/Ti₃C₂/Pt memristor in their study, utilizing inert Pt as the top electrode. The memristive behavior in this device was attributed to the reversible migration of oxygen vacancies within the Ti₃C₂ active layer, leading to the formation and rupture of conductive filaments [24].

Filamentary conduction, encompassing both ECM and VCM mechanisms, plays a pivotal role in the operation of MXene-based memristors. These mechanisms rely on the formation and dissolution of conductive filaments, driven by electrochemical redox reactions or the migration of atomic vacancies. Understanding these processes is crucial for designing and optimizing MXene-based memristive devices, paving the way for their application in next-generation memory and neuromorphic computing systems.

2.2.2 Charge trapping mechanism

The charge trapping mechanism is a fundamental process governing memristive devices, particularly those utilizing active materials with intrinsic charge trapping sites. Under an applied external voltage, charge carriers are gradually injected from the electrodes into these trapping sites within the active layer [25]. As the voltage increases, these traps sequentially become occupied, eventually reaching a critical threshold where the accumulated charges establish continuous transport pathways. This dramatically enhances the device's conductivity, facilitating the transition from a high-resistance state (HRS) to a low-resistance state (LRS). Conversely, applying a reverse voltage releases the trapped charge carriers, leading to the disintegration of conductive pathways. This reversible process allows the device to return to its initial HRS, demonstrating the characteristic bipolar resistive switching behavior. Recent advancements in materials science have highlighted several promising charge trapping materials for memristive applications, including MXenes, carbon nanotubes, metal nanoparticles (NPs), and fullerenes. These materials have exhibited remarkable potential in enhancing the performance and reliability of memristive devices through their efficient charge trapping capabilities. A notable demonstration of this mechanism was reported by Ding et al., who developed an Al/Ti₃C₂@polyvinylpyrrolidone (PVPy)/indium-tin-oxide (ITO) memristor exhibiting typical bipolar resistive switching characteristics [26]. Through a comprehensive analysis of current-voltage (I-V) characteristics using appropriate charge transport models, the researchers established the pivotal role of charge trapping in the resistive switching process.

The charge trapping mechanism in this device architecture involves the formation of conductive pathways (CPs) when the traps within the Ti_3C_2 layer reach full capacity, thereby triggering the transition from HRS to LRS. To further elucidate this phenomenon, Ding et al. employed advanced characterization techniques, including conductive atomic force microscopy (C-AFM). By analyzing CPs formed between the ITO electrode and AFM tips, along with current mapping images, the study provided conclusive evidence that the resistive switching behavior in Ti_3C_2 -based memristors is predominantly governed by the formation and rupture of CPs. Additionally, complementary characterization using Kelvin probe force microscopy (KPFM) was performed to validate the charge trapping and de-trapping processes under both positive and negative voltage biases. These measurements offered deeper insights into the charge-based switching mechanism, further reinforcing the understanding of the underlying physical processes.

The charge trapping mechanism presents a viable alternative to filamentary conduction in resistive switching devices (**Figure 1b**). By strategically engineering materials with optimized charge trapping properties, such as MXenes and their hybrid composites, researchers can significantly enhance the performance metrics and operational stability of memristive devices [25, 27]. This approach paves the way for the development of next-generation memory technologies and neuromorphic computing systems, offering innovative solutions for high-efficiency data storage and processing.

2.3 MXenes for multifunctional sensing and artificial intelligence applications

2.3.1 Artificial synapse

A synapse is the fundamental unit of neural communication, where two neurons connect to transmit information. Memristors, composed of top and bottom electrodes with a functional layer in between, structurally and functionally resemble biological synapses. By modulating resistance through ion migration—akin to the transmission of Ca^{2+} and Na^+ ions in biological synapses—memristors can replicate synaptic neurotransmission, making them promising candidates for artificial neural networks [28, 29]. A key property of synapses is plasticity, categorized into short-term and long-term synaptic plasticity. While traditional CMOS circuits have been used to simulate synaptic functions, their complexity and high energy consumption limit efficiency. Memristors, with their tunable conductance, offer a more efficient alternative for neuromorphic computing [30, 31].

Recent studies have demonstrated MXene-based memristors with synaptic behavior [11]. A $\text{Ti}_3\text{C}_2\text{T}_x$ -based memristor ($\text{Al}/\text{Ti}_3\text{C}_2\text{T}_x/\text{Pt}$) exhibited resistive switching, showing potentiation with 20 consecutive positive pulses and depression with 20 negative pulses (**Figure 2**). Zhao et al. developed an artificial synapse using oxidized MXenes as a floating gate tunneling layer, successfully replicating excitatory post-synaptic current (EPSC) and transitioning from short-term memory to long-term memory, consistent with Ebbinghaus' forgetting law. Wang et al. fabricated an $\text{Ag}/\text{V}_2\text{C}/\text{W}$ memristor capable of both threshold and resistive switching by adjusting compliance current (ICC). The device mimicked calcium ion flux, exhibited PPF behavior, and demonstrated STDP, with larger spike time differences resulting in smaller synaptic weight changes. These advancements in MXene-based memristors highlight their potential for neuromorphic computing, offering energy-efficient and biologically inspired solutions for artificial neural networks.

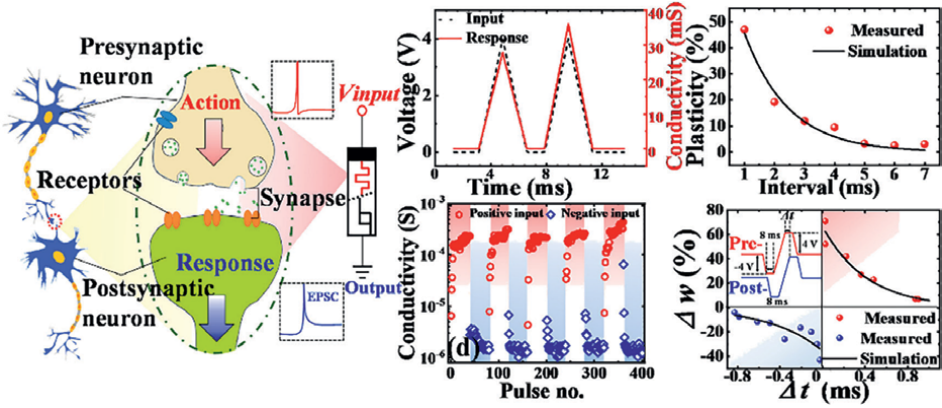


Figure 2. The emulation of synaptic learning. The conductivity responses, potentiation/depression (blue) epochs, and STDP learning rules [11].

2.3.2 Logic circuit

Logic circuits execute operations based on defined relationships between input signals, with fundamental gates such as NOT, OR, AND, and NAND [32]. Traditional computing architectures require separate memory and processing units, leading to increased energy consumption and computation time. In contrast, RRAM enables in-memory computation with parallel processing, significantly improving efficiency. However, its binary-state limitation constrains advanced logic applications, necessitating multivalued storage or multifold coupling for enhanced functionality. To address these challenges, researchers developed an optoelectronic RRAM using silver nanoparticle (Ag NP)-doped $\text{TiO}_2/\text{MXene}$ nanosheets (AMT) [33]. Regulating Ag NP concentration and MXene oxidation time *via* a hydrothermal oxidation process, they achieved a 0.5 V SET voltage and nonvolatile bipolar resistive switching. The intermediate resistive state was modulated by ultraviolet light, while the SET voltage was tunable through Ag NP density. This work demonstrates the feasibility of integrating optoelectronic data storage with logic operations and advancing MXene-based optoelectronic circuits.

While traditional memristors have enabled decimal computations, research on 2D material-based memristors for such applications remains limited. Wang et al. introduced Ag decorating to enhance the neuromorphic performance of Ti_3C_2 -based memristors [34]. This approach mitigated Ag electrode dissolution and abrupt current transitions in pure Ti_3C_2 devices, enabling smooth, bidirectional resistive switching. The device exhibited linear resistive transitions under both positive and negative voltage stimuli. These findings underscore the potential of metal nanoparticle doping in improving Ti_3C_2 memristors and advancing neuromorphic computing.

The integration of MXene with oxide-based memristors harnesses its exceptional electrical and optical properties to enhance device performance, advancing neuromorphic hardware. This study focuses on improving weight update behavior by incorporating MXene into yttrium-doped hafnium dioxide (Y:HfO_2) memristors [35]. The resulting MXene/ Y:HfO_2 artificial synapses emulate key biological functions. Additionally, the device exhibits a strong photoelectric

response, enabling synaptic weight modulation under light stimulation. A photoelectric logic gate circuit was further developed, highlighting the potential of MXene/Y:HfO₂ synapses for optoelectronic neuromorphic computing and logic applications. Moreover, a near-infrared (NIR)-responsive MXene@MAPbI₃-based RRAM was developed *via* a simple dip-coating process [36]. Under 1064-nm laser illumination (within the tissue optical window), the device demonstrated a reduced SET voltage of +1.30 V compared to +2.16 V in the dark (**Figure 3c**). This NIR-controlled switching enables in-memory logic operations such as “AND,” “OR,” and “NOT,” with potential applications in biocompatible RRAM microchips for *in vivo* control and artificial neuromorphic vision. These fibrous resistive switching devices hold promise for next-generation e-textiles, integrating digital storage and information processing.

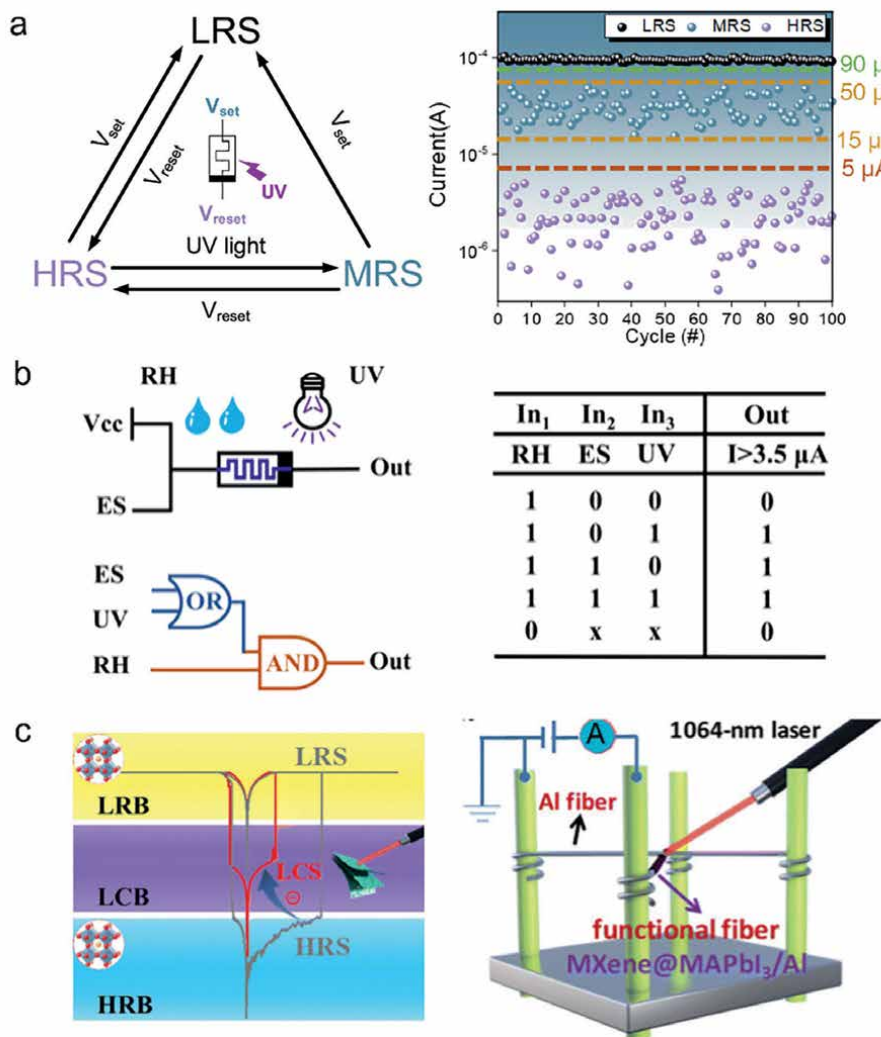


Figure 3.
(a) Operating input factors and current changes during transition processes [33]. (b) Photoelectric memristor and truth table of AND and OR operations [34]. (c) Light-controlled state in the Al/MXene@MAPbI₃/Al device [36].

2.3.3 Neuromorphic computing

As the exponential growth of information, traditional computing faces increasing constraints due to the memory wall resulting from the von Neumann architecture. Neuromorphic computing has emerged as an alternative, mimicking the efficient information processing of biological neural networks. Among recent advancements, MXene-based memristors have demonstrated significant potential in in-memory computing.

Yan et al. utilized $\text{Ti}_3\text{C}_2\text{T}_x$ MXene becoming the active layer, where oxygen vacancies and Ti used as charge trap sites, enabling synaptic functions [11]. Wei et al. integrated a lithium-polymer-electrolyte with Ti_3C_2 MXene, leveraging its ion diffusion to facilitate lithium-ion migration, enabling multistate conductivity control [37]. However, despite reports of resistive switching in MXene layers, essential synaptic characteristics including linear long-term depression (LTD)/long-term potentiation (LTP), multiple conductance states, and high on/off ratios remain underexplored. Ju et al. fabricated an artificial $\text{Ti}_3\text{C}_2\text{T}_x$ MXene-based synapse that successfully emulates key biological synaptic dynamics. Their study demonstrated the effectiveness of MXene synapses in neural networks using the CIFAR-10 dataset (**Figure 4a**).

Flexible hardware neural networks hold significant promise for next-generation wearable electronics. A PET/ITO/p-MXene/Ag flexible memristor was developed by regulating aluminum ion etching in $\text{Ti}_3\text{C}_2\text{T}_x$ MXene. This device exhibited high mechanical stability under bending angles up to $\sim 73^\circ$ and environmental robustness under varying temperature and humidity conditions (**Figure 4b**) [38]. Furthermore, CNN-based simulations achieved a remarkable $\sim 95\%$ accuracy in recognizing modified MNIST patterns within just 29 training epochs, highlighting the potential of MXene-based flexible memristors [39]. In addition, adaptive weight adjustment is crucial for high-accuracy neuromorphic devices. To address this, researchers

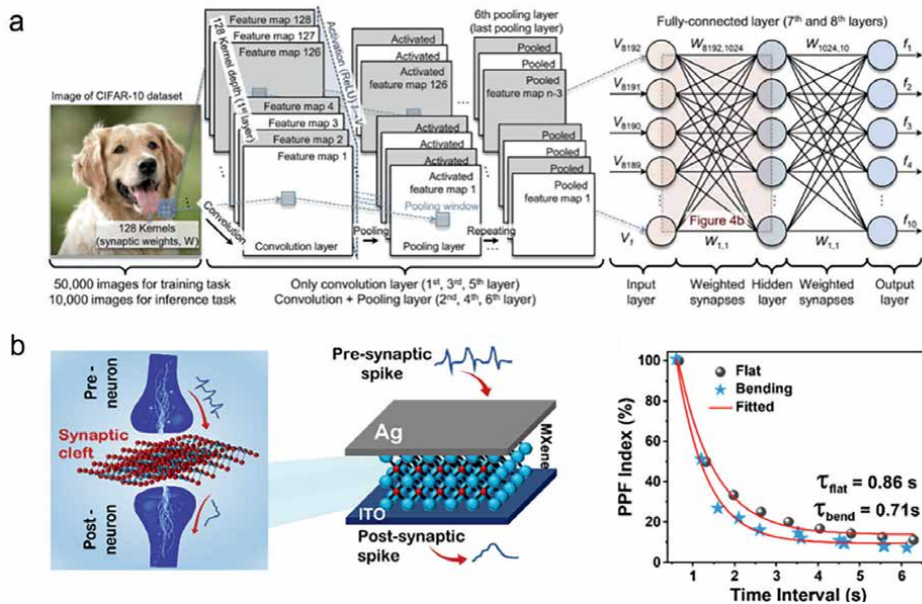


Figure 4. (a) Neural network based on MXene devices [37]. (b) Bending test for MXene synapses [38].

developed self-adaptive artificial synapses based on flexible and tunable MXene-based energy storage devices. Training and machine learning evaluations demonstrated that the device achieved a 95% recognition accuracy [40].

2.3.4 Multimodal in-sensor computing

In-sensor computing, where interconnected sensing devices process information, has become a potential approach to enhance the energy, area, and time efficiency of artificial intelligence [41–47]. Human vision, for instance, is highly influenced by environmental conditions such as extreme relative humidity (RH), necessitating intelligent devices capable of sensing-dependent signal processing to adapt to changing environments. Current research primarily focuses on single-sensing processing (**Figure 5a**). However, human sensing ability integrates multiple sensory inputs simultaneously to navigate complex environments. Addressing this challenge, an MXene-ZnO memristor with multiple senses has been designed to emulate the human eye, integrating RH sensing, visual data sensing, and information preprocessing functions [41]. By reducing the complexity of traditional neuromorphic vision systems, this approach advances device-level intelligence for real-world applications (**Figure 5b**).

To maintain high device functionality while avoiding the adverse effects of high-temperature processing, low-temperature fabrication techniques are essential for reliable integrated systems. MXene nanosheets, with their exceptional conductivity and adjustable surface functional groups, offer great potential for developing highly flexible memristor arrays. An integrated MXene-based flexible sensory device has been developed using an energy-efficient, room-temperature oxidation process [48]. This MXene-based sensor-memristor system achieved high-precision human motion decisions and recognition of handwritten digits, demonstrating real-time monitoring potential *via* sensor-collected signals processed through artificial neural networks (**Figure 5c**).

Despite significant research on MXene synthesis for various applications, the fabrication process introduces variability in surface terminations, defects, and interlayer spacing. While these factors allow for tunable properties, they also pose challenges for device reproducibility. Additionally, current deposition techniques, though cost-effective, often lead to incomplete surface coverage and variability, which impact resistive switching mechanisms [49]. Modifying MXene flakes is a common strategy to enhance their physicochemical properties. Similar approaches are now being applied to MXene-based memristors, including nanoparticle doping and induced oxidation, which improve retention, endurance, and forming-free behavior. However, these modifications alone do not fully address the high conductivity of MXenes, which limits their neuromorphic capabilities. A more holistic tuning approach is needed when using MXenes as the sole RS layer in neuromorphic electronics. MXene-based memristors can successfully mimic fundamental synaptic functions but still lag in key functions required for complex neuromorphic computing. Endurance is a critical factor—filamentary switching significantly impacts device lifespan. Eliminating the forming process would prevent structural changes that degrade endurance. Both linearity and symmetry are crucial for precise synaptic weight updates, but these are heavily influenced by filamentary switching dynamics. Strategies to improve these characteristics are needed. Future designs should incorporate sensors to enable multimodal in-sensing-memory-computing for more biologically realistic neuromorphic systems. Key future research directions include developing large-scale, reproducible

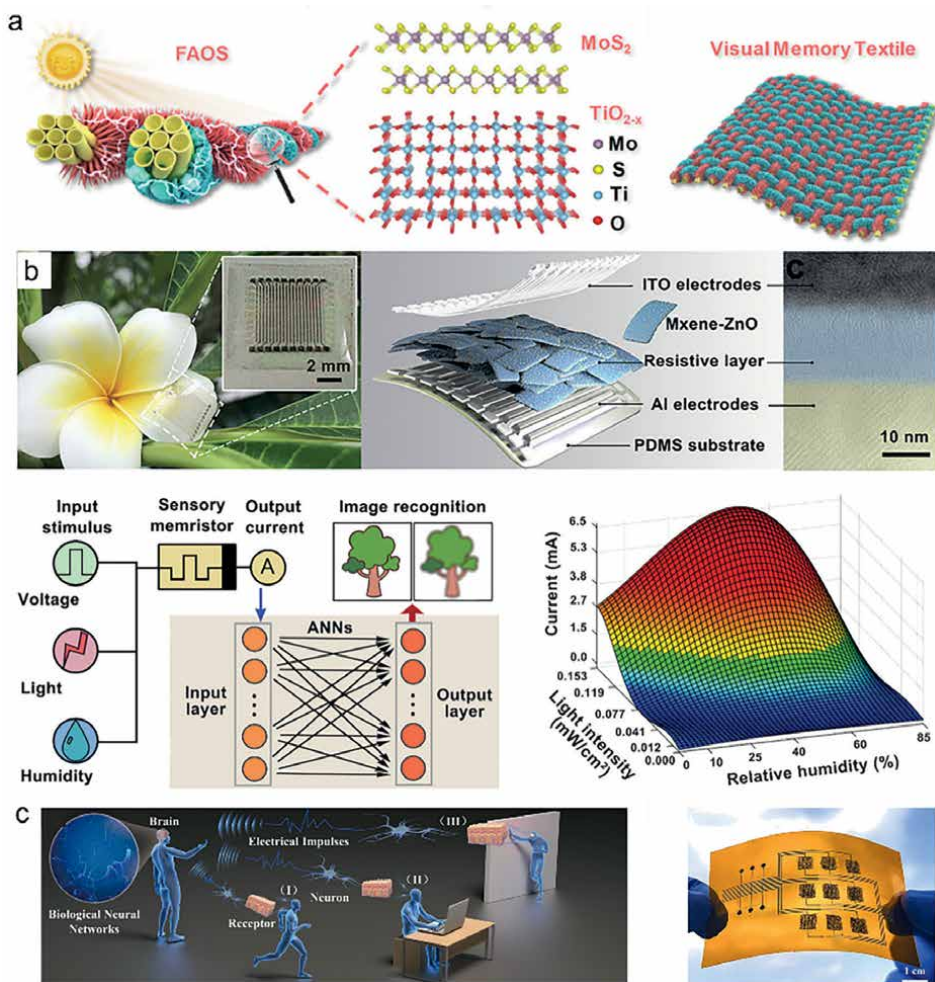


Figure 5. (a) Schematic representation of photoelectric synapses in flexible fibers [42]. (b) Photograph of the flexible MXene based devices [41]. (c) Photograph of sensory-processing system [48].

synthesis and deposition techniques; exploring alternative RS mechanisms beyond filamentary switching; enhancing environmental stability through functionalization strategies; improving endurance, linearity, and forming-free behavior; and integrating MXene-based sensors with neuromorphic computing for real-time perception and processing. These advancements will offer a pathway for MXene memristors to play a crucial role in next-generation artificial intelligence hardware.

3. Conclusions

Neuromorphic devices, particularly memristors, have emerged as a promising alternative, offering scalable, high-speed, and low-power computing capabilities that address the limitations imposed by the von Neumann architecture. Among various materials explored for neuromorphic applications, two-dimensional MXenes stand out due to their exceptional mechanical and electrical properties. These materials

provide significant advantages in sensing, nonvolatile memory, and bio-inspired computation, making them a transformative platform for next-generation neuromorphic devices. Advances in MXene synthesis and device fabrication have enabled the development of flexible memristor-based neuromorphic architectures, integrating memory, computation, and multimodal sensing functionalities. Despite remarkable progress, challenges remain in ensuring the stability, scalability, and interfacial optimization of MXene-based devices. Future research should pay attention to improving device endurance, optimizing switching mechanisms, and integrating MXene-based architectures into fully functional sensing-memory-processing networks. The continued advancement of MXene-integrated systems holds immense potential to revolutionize AI hardware, enabling more adaptive, energy-efficient, and scalable computing paradigms beyond the limitations of traditional architectures.

Conflict of interest

The authors declare no conflict of interest.

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Application of MXenes-Based Materials in Biomedical Engineering

Shisheng Cui, Yingyan Wu, Chengli Ni and Haili Wang

Abstract

MXenes-based composite materials, as emerging two-dimensional materials, have shown extensive potential in the biomedical field due to their excellent electrical, mechanical, and surface properties. MXenes possess diverse surface chemistry that enables interactions with a variety of biomolecules, promoting innovations in drug delivery, cellular imaging, cancer therapy, and more. By combining MXenes with various biomaterials such as polymers, metal nanoparticles, and carbon materials, their performance is further enhanced, improving biocompatibility, stability, and functionality. These composite materials have demonstrated significant promise in cancer-targeted therapy, tissue engineering, sensor development, and antimicrobial treatment. This chapter summarizes the latest advancements in the biomedical applications of MXenes-based composites and discusses the challenges and future directions for their development.

Keywords: MXenes, drug delivery, biosensing, antimicrobial properties, tissue regeneration, biomedical applications

1. Introduction

MXenes, a family of two-dimensional (2D) materials first discovered in 2011, have attracted considerable attention due to their unique properties [1], including high conductivity, mechanical strength, hydrophilicity, and surface chemistry, that allows for the modification of their physical and chemical characteristics [2]. Composed of transition metal carbides, nitrides, or carbonitrides, MXenes possess a layered structure similar to graphene, but with additional metal-based elements that give them distinct advantages in various applications. As an important member of the two-dimensional material family [3], MXenes have shown great application potential in many fields since its discovery by virtue of its excellent physical and chemical properties, especially in the biomedical field, is gradually emerging [4].

The biomedical field, with its demands for multifunctional materials, has seen rapid exploration of MXenes and their composites for a wide range of applications [5]. MXenes can be easily functionalized with bioactive molecules, enhancing their ability to interact with biological systems [6]. This makes them ideal candidates for applications in drug delivery, biosensors, cancer treatment, tissue engineering, and antimicrobial

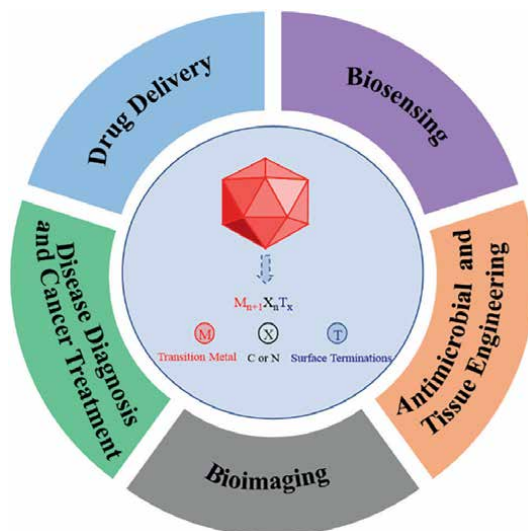


Figure 1.

The structure of this chapter, including the MXene structure, application of MXenes in drug delivery, biosensing, antimicrobial therapies, tissue engineering, bioimaging, disease diagnosis, and cancer treatment.

therapies. However, while MXenes themselves offer numerous benefits, their properties can be further optimized when integrated with other materials, forming composites that combine the strengths of each component [7]. For example, MXenes incorporated into polymer matrices, metal nanoparticles, or carbon-based materials can provide synergistic effects that improve stability, biocompatibility, and performance in complex biological environments [8].

This chapter provides a comprehensive overview of the advancements in MXenes-based composite materials for biomedical applications, including drug delivery, biosensing, antimicrobial therapies, tissue engineering, bioimaging, disease diagnosis, and cancer treatment (**Figure 1**) [9]. It will cover the key design and synthesis methods of these composites, while also addressing the challenges they encounter and the future directions of research. The goal is to offer insights and guidance for further studies and practical applications in this area [10].

2. Application of MXenes-based materials in drug delivery

Drug delivery systems are a key focus in modern medical research, aiming to precisely and efficiently transport drugs to targeted sites, enhance therapeutic efficacy, and minimize harmful side effects. Traditional delivery methods often suffer from issues such as low drug utilization and inadequate targeting. MXenes, with their distinctive physical and chemical properties, offer significant advantages for drug molecule loading and adsorption, showing great promise in advancing drug delivery technologies [11]. In recent years, the use of MXene composites in drug delivery has garnered increasing attention, offering innovative approaches to the development of more effective systems. Research indicates that 2D Ti_3C_2 (titanium carbide) MXene, in particular, holds great potential as a drug delivery agent. Its unique biological activity, ultra-thin two-dimensional structure, and ability to easily traverse blood vessels make it a valuable tool in chemotherapy and in the complete eradication of tumors [12].

Han et al. developed a novel approach to functionalize and modify the surface of Nb₂C MXenes, creating a “therapeutic mesopore.” Unlike traditional methods that load chemical drugs into mesopores, their approach preserves the mesopore-forming agent within the mesopores, eliminating the need for additional chemotherapy drugs [13]. This innovation bypasses the complex steps of surfactant extraction and drug loading, while still achieving a high drug loading capacity (32.57%). Additionally, targeted modification is accomplished through RGD coupling, allowing selective recognition of the $\alpha v \beta 3$ integrin, which is overexpressed on cancer cell membranes. When exposed to 1064-nm laser irradiation, the 2D Nb₂C core within the composite nanosheet exhibits strong photoresponsiveness and excellent photothermal conversion efficiency ($\eta = 28.6\%$). Both *in vitro* and *in vivo* experiments demonstrated that these “therapeutic mesopore”-coated Nb₂C nanosheets significantly enhanced the treatment of U87 brain cancer cells (Figure 2).

Xing et al. were the first to successfully synthesize a composite hydrogel combining cellulose and Ti₃C₂ MXene [14]. Their study revealed that the cellulose/MXene hydrogel exhibits a rapid and continuous response to near-infrared (NIR) light. This property enables a significant acceleration in the release rate of the anticancer drug doxorubicin hydrochloride (DOX) when loaded into the hydrogel. The enhanced release is due to the expansion of pores in the three-dimensional cellulose network,

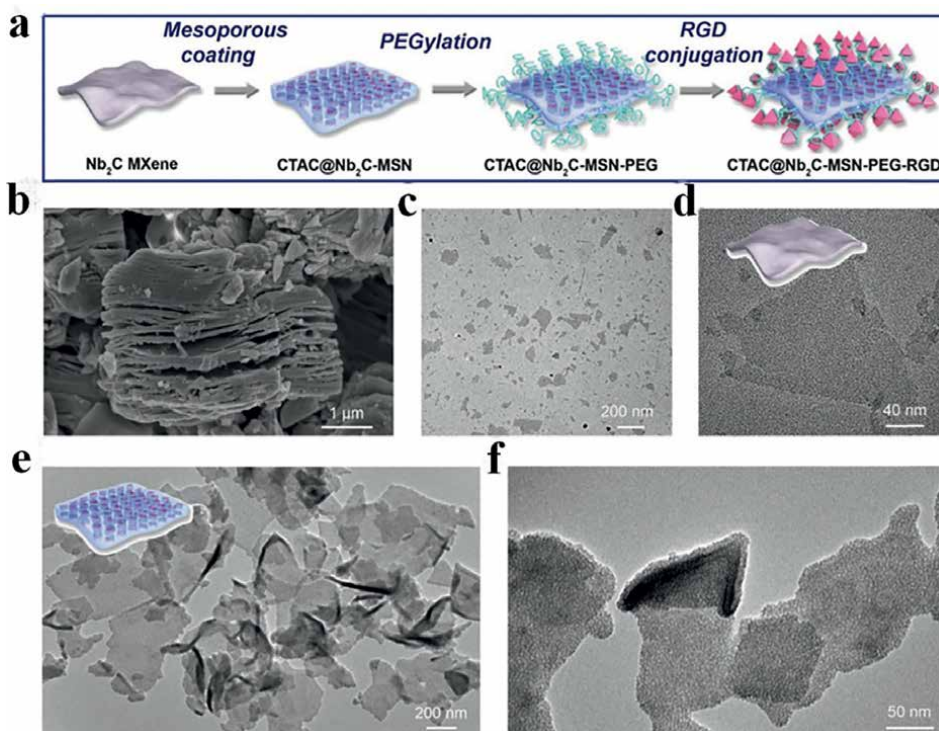


Figure 2.
 The CTAC@Nb₂C-MSN nanosheets with core-shell structure synthesized based on Nb₂C MXene. (a) Synthesis process of CTAC@Nb₂C-MSN nanosheets and targeted modification process of PEGylation. (b) SEM image of Nb₂C MXene synthesized by HF acid etching in the first step. (c) Images of Nb₂C MXene nanosheets under transmission electron microscope at low magnification and (d) high magnification. (e) Images of CTAC@Nb₂C-MSN composite nanosheet under transmission electron microscope at low magnification and (f) high magnification [13].

triggered by 808-nm light irradiation. With its excellent photothermal performance and controlled drug release, the cellulose/MXene hydrogel serves as a multifunctional nanoplatform for intratumoral drug delivery. The results demonstrate that the combination of photothermal therapy and chemotherapy using this nanoplatform effectively destroys tumors and inhibits recurrence, highlighting its potential in cancer treatment applications.

Thermally responsive wound dressings have garnered significant attention for their ability to monitor conditions in real time and deliver drugs on demand. However, effective systems for precise temperature control and regulated drug release are still lacking. Cheng et al. addressed this gap by designing an intelligent fabric for wound management that integrates thermally responsive drug delivery with temperature monitoring [15]. The system consists of three layers: a drug-loaded thermosensitive nanofiber membrane, an MXene-enhanced Joule heating membrane, and an FPCB control chip. By applying a low voltage (0–4 V) to the heating membrane, the system maintains stable temperature stimulation ranging from 25–130°C, with real-time monitoring and adjustment capabilities. This low-voltage Joule heating ensures precise control, allowing the drug-loaded membrane to release its therapeutic agents in response to temperature changes. *In vitro* tests show significant antibacterial effects, while *in vivo* experiments confirm that the fabric promotes wound healing and accelerates recovery.

In cancer treatment, two-dimensional MXene nanomaterials are promising, particularly for photothermal therapy, but their use as drug carriers remains

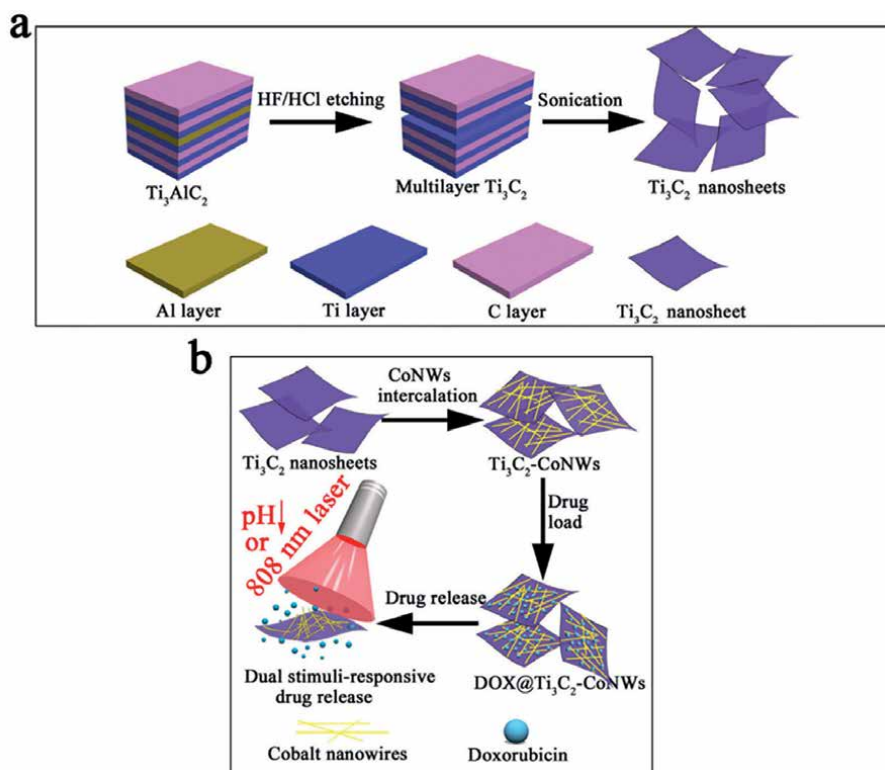


Figure 3. (a) Schematic diagram of the synthesis of Ti_3C_2 nanosheets. (b) Flow chart of the dual stimulus responsive drug release after the combination of Ti_3C_2 nanosheets and CoNWs and loading with DOX [16].

challenging due to difficulties in precise control. To address this, Liu et al. developed a heterostructured titanium carbide-cobalt nanowire ($\text{Ti}_3\text{C}_2\text{-CoNWs}$) nanocarrier with magnetic control, dual stimulus-responsive drug release, and combined chemo-photothermal therapeutic functions for enhanced cancer treatment (**Figure 3**) [16]. The study examined the nanocarrier's structure, drug loading/release behavior, magnetic control, and photothermal performance, revealing exceptional photothermal conversion efficiency under 808-nm laser irradiation. The nanocarrier demonstrated a high drug loading capacity of 225.05%, with drug release triggered by acidic pH or near-infrared radiation. Compared to chemotherapy or photothermal therapy alone, the combined approach using the heterojunction nanocarrier proved more effective in inducing cancer cell death, making it a promising option for improving cancer treatment outcomes.

3. Application of MXenes-based materials in biosensor

3.1 Detection of biomacromolecules

Biosensing technology plays a key role in the fields of medical diagnosis, food safety, and environmental monitoring, and accurate, fast, and efficient biosensing technology is an important guarantee for the effective detection of biological substances [17]. As a new type of two-dimensional material, MXenes also shows great development potential in the field of biosensing with its unique physical and chemical properties [18].

When it comes to biomolecular detection, MXenes materials show excellent performance. Ochratoxin A (OTA) is highly susceptible to food contamination and poses a significant threat to human health. To enable accurate detection and timely warning of OTA contamination, Liu et al. presents a novel four-mode nanobiosensor detection system based on MXenes (**Figure 4**) [19]. The V_2C nanomaterial ($\text{V}_2\text{C-NMS}$), which exhibits strong fluorescence quenching properties, was synthesized using a combination of *in situ* chemical etching, metal ion insertion, and collaborative physical stripping techniques. Following adaptor functionalization, $\text{V}_2\text{C-NMS}$ was conjugated with single-stranded DNA (ssDNA) to form $\text{V}_2\text{C-NMS@ssDNA}$, which demonstrated excellent peroxidase-like activity. This enabled the development of an OTA fluorescence/colorimetric biosensor, where the fluorescence and colorimetric signals exhibited a strong linear correlation with OTA concentration, achieving a detection limit as low as 6.77 pg./mL. In addition, a fully connected artificial neural network (FCANN) was created using RGB values from the fluorescence/colorimetric biosensor, allowing for rapid prediction of OTA concentrations in samples within seconds, with a detection limit of 7.10 pg./mL. The four-mode approach showed excellent performance in real sample analysis, with recovery rates ranging from 95.33 to 105.79%. The results from the four modes were consistent and mutually verified.

Manganese dioxide nanosheets (MnO_2 NSs) have gained significant attention in biomedical sensing; however, their preparation often involves complex processes, including the use of reducing agents, templates, or high temperatures. Yi et al. proposed a simpler, one-step approach to assemble a new $\text{Ti}_3\text{C}_2\text{T}_x$ MXene nanoribbon modified with MnO_2 NSs ($\text{Ti}_3\text{C}_2\text{T}_x\text{NR@MnO}_2$), which serves as a dual signal generator for colorimetric and fluorescence (FL) sensing (**Figure 5**) [20]. In this assembly, $\text{Ti}_3\text{C}_2\text{T}_x\text{NR}$ acts both as a reducing agent and a stabilizing carrier, preventing aggregation of the MnO_2 NSs. The strong interaction between $\text{Ti}_3\text{C}_2\text{T}_x$ and MnO_2 enhances

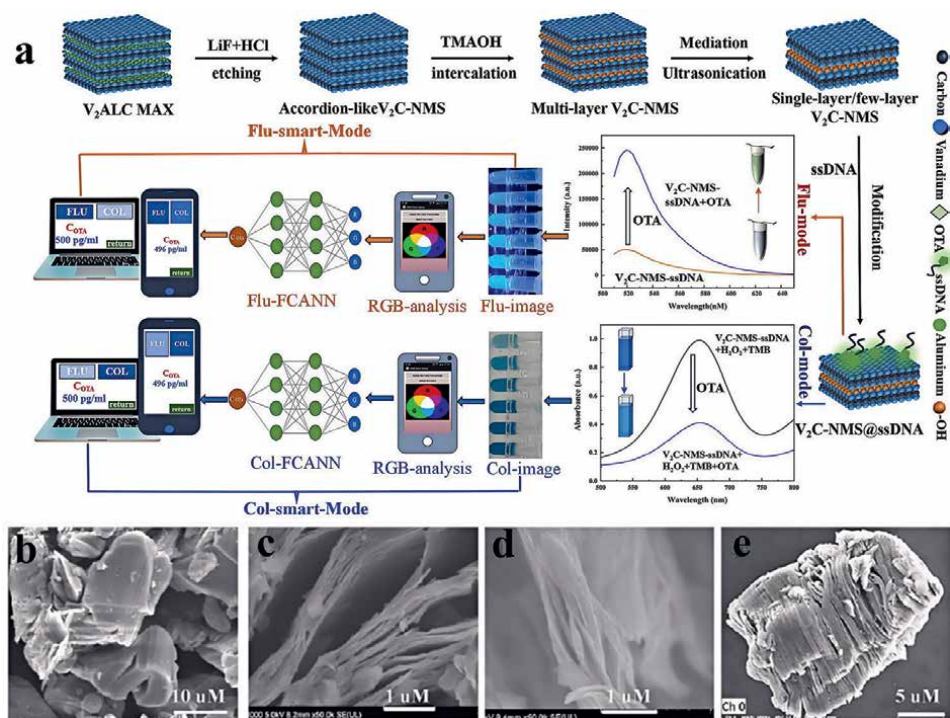


Figure 4.

(a) Construction method and OTA detection principle of V₂C-NMS four-mode nanobiosensor system. (b) SEM image characterization of MAX phase V₂AlC, and (c-e) SEM image of V₂C MXenes [19].

the oxidase-like activity and oxidation properties of the composite. The performance of 3,3,5,5-tetramethylbenzidine (TMB) and thiamine (TH) was evaluated to assess the system's activity and oxidation capabilities. In the absence of dichlorvos (TCF), the MnO₂ coating on Ti₃C₂T_xNR specifically recognizes thiocholine (TCh), a product of acetylcholinesterase (AChE)-catalyzed hydrolysis of acetylthiocholine. This recognition leads to the breakdown of MnO₂ into Mn²⁺, resulting in a reduction of both the colorimetric and fluorescence signals. The strong interaction between Ti₃C₂T_x and MnO₂, along with the specific recognition of TCh, significantly enhances the sensitivity of the dual-mode sensor. The detection limits for colorimetry and fluorescence were 0.0856 and 0.798 ng/mL, respectively. This approach offers a novel strategy for constructing multifunctional probes and enables efficient, accurate biosensing detection.

3.2 Detection of disease marker

In the field of disease diagnosis, MXenes materials have important applications in the detection of disease markers. For the detection of tumor markers, the researchers used the MXenes material's high specific surface area and good electrical conductivity to build immune sensors [21]. By fixing the specific antibody on the surface of the MXenes-modified electrode, when there are tumor markers in the sample, the antibody binds specifically to the tumor markers, causing changes in the electrical properties of the electrode surface. By detecting such changes, highly sensitive detection of tumor markers can be achieved [22].

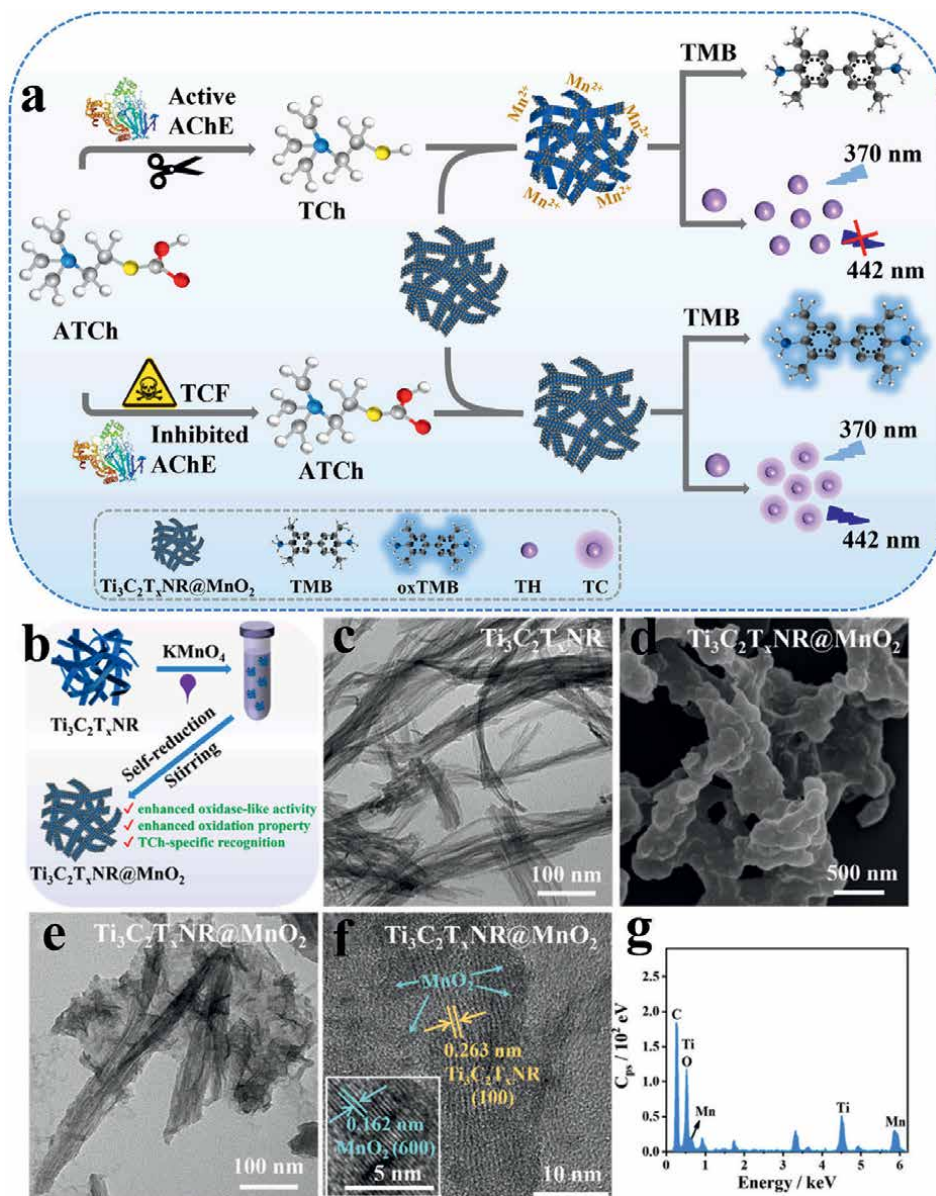


Figure 5.
 (a) Schematic diagram for TCF detection sensor. (b) Schematic illustration of the manufacturing process of $\text{Ti}_3\text{C}_2\text{T}_x\text{NR}/\text{MnO}_2$. (c) TEM image of $\text{Ti}_3\text{C}_2\text{T}_x\text{NR}$. (d) SEM image of $\text{Ti}_3\text{C}_2\text{T}_x\text{NR}/\text{MnO}_2$. (e) TEM image of $\text{Ti}_3\text{C}_2\text{T}_x\text{NR}/\text{MnO}_2$. (f) HRTEM image of $\text{Ti}_3\text{C}_2\text{T}_x\text{NR}/\text{MnO}_2$. (g) EDS analysis [20].

The level of carcinoembryonic antigen (CEA) in serum is strongly linked to colorectal cancer, making its rapid and efficient detection crucial. Lei et al. developed a simple, low-cost, and environmentally friendly template-assisted filtration method to prepare scalable carbon nanotube-bridged $\text{Ti}_3\text{C}_2\text{T}_x$ MXene (MX@CNT) electrode arrays with conductive networks [23]. They used this to construct a homogeneous electrochemical (HEC) sensor for CEA detection, employing a magnetic bead-based alkaline phosphatase-linked immunoassay (MB-aELISA) that generates the

electroactive substance 1-naphthol (1-NP) *in situ*. The MX@CNT electrode array's unique electrochemical properties—such as its ultra-low background signal and high electrocatalytic activity for hydrolyzed 1-NP—enhance the sensor's performance. This enables the MB-aELISA-based HEC sensor to detect CEA within a range of 0.005 to 1.0 ng/mL, with a detection limit as low as 1.6 pg./mL. *In vivo* experiments demonstrated that the biosensor prototype successfully detected CEA in serum samples from patients with colorectal cancer.

The detection of the tumor marker carbohydrate antigen 125 (CA125) can be enhanced through a bimetallic organic framework (MOF) sandwich strategy. Qu et al. present a versatile approach to synthesizing homogeneous MXene and MIL-101(Fe)-NH₂ composites, leveraging the strengths of both materials [24]. MXene offers excellent electrical conductivity and a high surface area, while mesoporous MIL-101(Fe)-NH₂ enhances the loading capacity for the primary antibody and provides catalytic activity through its iron (Fe) metal centers. Additionally, UiO-66 modified with methylene blue (MB) serves as an electrochemical immunosensor signal tag for CA125 detection. This immunosensor demonstrates high sensitivity and a low detection limit (LOD) of 0.006 U/mL, offering a promising method for the early diagnosis of CA125.

4. Application of MXenes-based materials in antimicrobial therapy and tissue engineering

4.1 MXenes-based materials in antimicrobial therapy

The growing demand for new materials in the biomedical sector highlights the importance of research and development aimed at addressing antibacterial challenges and enhancing tissue repair and regeneration [25]. Among the promising materials, MXenes have garnered significant attention due to their unique structure and versatile properties. In particular, their potential in antibacterial applications and tissue engineering makes them an exciting prospect for advancing treatments for related diseases and promoting tissue regeneration.

The antibacterial mechanisms of MXenes can be categorized into three main effects. First, the physical damage effect: MXenes' two-dimensional sheet structure, with sharp edges and a large specific surface area, allows direct interaction with bacterial cell membranes. This mechanical interaction disrupts the membrane's integrity, causing the leakage of cellular contents and ultimately leading to bacterial cell death. Second, the oxidative stress effect: MXenes can generate reactive oxygen species (ROS) and hydroxyl radicals in physiological environments. These ROS possess strong oxidizing capabilities, enabling them to damage essential biological macromolecules—such as proteins, nucleic acids, and lipids—within bacterial cells, thereby impairing cell function and contributing to the antibacterial effect. Finally, the electrostatic interaction: MXenes surfaces are typically negatively charged under physiological conditions, while bacterial cell membranes often contain positively charged sites. Through electrostatic attraction, MXenes can bind to these sites, disrupting the charge balance of the bacterial membrane. This increases membrane permeability and ultimately causes bacterial cell death.

By adding MXenes material to traditional dressing materials, a composite dressing with antibacterial properties can be prepared. The antibacterial properties of MXenes material can effectively inhibit the growth and reproduction of bacteria on the wound

surface, reduce the occurrence of infection, and promote wound healing. Titanium carbide (MXene) is known for its antibacterial properties, which include the ability to damage bacterial membranes physically and induce oxidative stress chemically. Zheng et al. developed a synergistic antimicrobial agent by attaching ultra-small gold nanoclusters (AuNCs) to MXene nanosheets (**Figure 6**) [26]. Following bacterial membrane damage by MXene, the AuNCs are efficiently delivered to the bacteria, generating high levels of local ROS that contribute to bacterial death. This combined

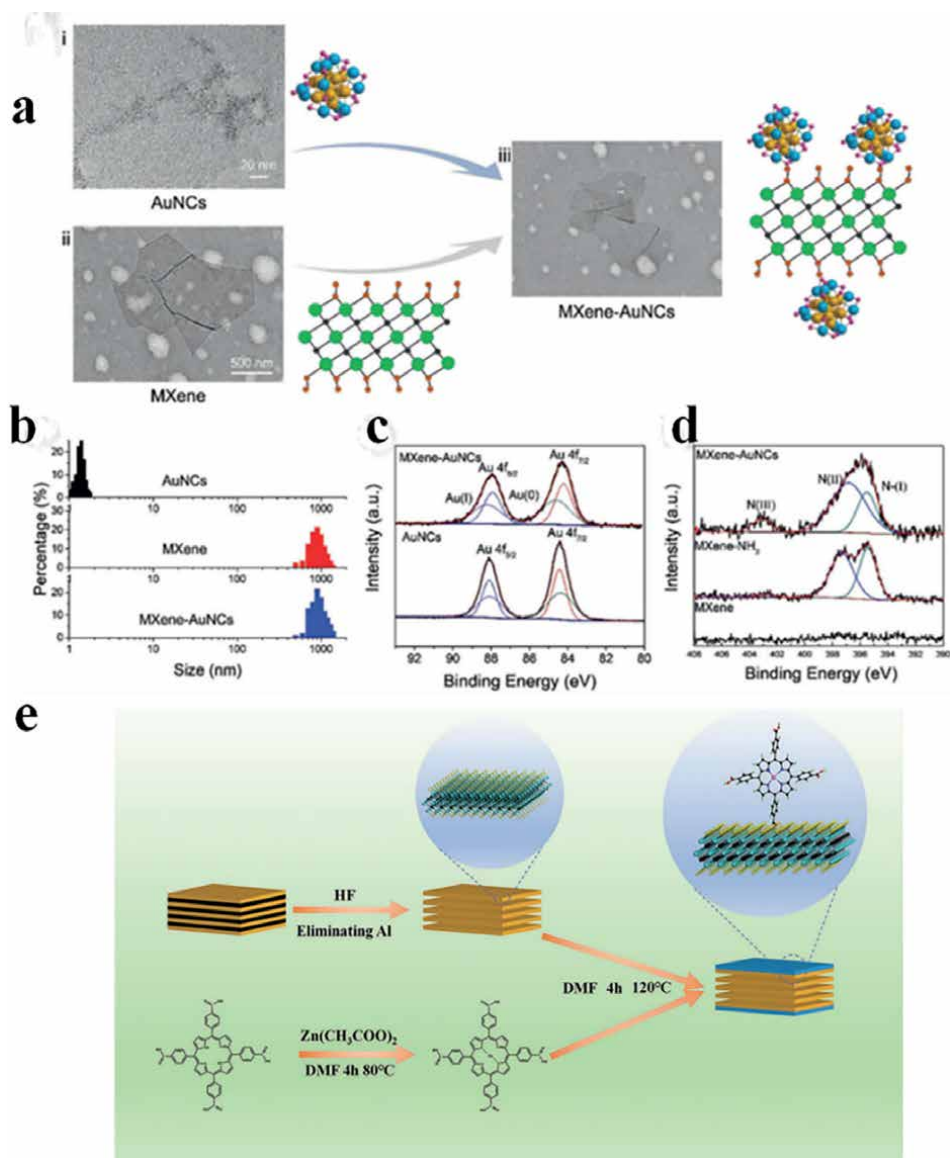


Figure 6. (a) Representative TEM images of AuNCs, MXene, and MXene-AuNCs. (b) Size distributions of AuNCs, MXene, and MXene-AuNCs. (c) X-ray photoelectron spectroscopy (XPS) results of Au element of MXene-AuNCs and AuNCs. (d) XPS results of N element of MXene-AuNCs, MXene-NH₂, and MXene. (e) Synthesis mechanism diagram of ZnTCPP/Ti₃C₂T_x [26].

physical (*via* MXene) and chemical (*via* MXene and AuNCs) mechanism effectively targets both Gram-positive and Gram-negative bacteria. Additionally, the crumpled MXene-AuNCs structure prevents biofilm formation. The binding of MXene and AuNCs, along with the structure's hydrophobic surface, inhibits bacterial attachment, while its large surface area enhances the overall antibacterial efficacy.

Photoassisted antimicrobial therapy offers a promising alternative to traditional antibiotic treatments, as it provides high antimicrobial efficacy without leading to bacterial resistance. Cheng developed a visible-light-responsive ZnTCPP/Ti₃C₂T_x organic-inorganic hybrid that can effectively treat bacterial infections within just 10 minutes [27]. This hybrid demonstrates exceptional antibacterial efficiency, achieving 99.86 and 99.92% effectiveness against *Staphylococcus aureus* and *Escherichia coli*, respectively. Both *in vitro* and *in vivo* studies show that ZnTCPP/Ti₃C₂T_x exhibits outstanding antibacterial properties when exposed to visible light, thanks to its superior bactericidal and photocatalytic effects.

4.2 MXenes-based materials in tissue engineering

MXenes material has good biocompatibility and can provide a suitable microenvironment for cell adhesion and proliferation. The electrical conductivity of MXenes materials can also regulate the physiological function of cells through electrical stimulation, and promote cell proliferation and differentiation. Studies have shown that adding MXenes materials to tissue engineering scaffolds can significantly improve the adhesion and proliferation ability of cells on the scaffolds, providing a good cellular basis for tissue repair and regeneration. In tissue engineering, MXenes materials can induce differentiation of stem cells by regulating physical and chemical signals in the cell microenvironment. For example, in bone tissue engineering, MXenes materials can promote the differentiation of bone marrow mesenchymal stem cells into osteoblasts, enhance the osteogenic activity of the cells, and promote the formation and repair of bone tissue. Wu et al. developed a near-infrared light-responsive hydrogel system designed to facilitate programmed tissue repair and regeneration [28]. The hydrogel, referred to as HG/MPa, is composed of hydroxypropyl chitosan/gelatin (HG) modified with Ti₃C₂T_x MXene nanosheets (MP) that are further coated with polydopamine and acid fibroblast growth factor (aFGF). This system effectively coordinates bone vascular network reconstruction and supports bone regeneration. When exposed to near-infrared light, the HG/MPa hydrogel releases aFGF, stimulating rapid angiogenesis and improving blood supply. The integrated hydrogel system also promotes cell adhesion and proliferation following regular near-infrared irradiation. *In vivo* studies demonstrate that this time- and space-controlled hydrogel platform works synergistically with photothermal therapy, enhancing the production of osteogenic and angiogenic factors and accelerating bone defect healing.

5. Application of MXenes-based materials in bioimaging

Bioimaging technology is very important in modern medical research and clinical diagnosis, which can realize the visual monitoring of the changes of structure, function, and molecular level in organisms without damaging biological tissues [29]. With the rapid development of nanotechnology, new nanomaterials continue to emerge, which provides a new opportunity for the progress of bioimaging technology. MXenes materials have attracted the attention of many researchers because of their excellent

electrical, optical, and thermal properties. It has good thermal and chemical stability, and can exist relatively stably in organisms, so it has great potential as a biological imaging probe [20].

5.1 Fluorescence imaging

Fluorescence imaging has the advantages of high sensitivity, high resolution, and real-time monitoring. MXenes materials can be combined with fluorescent molecules to construct composite fluorescent probes by means of surface modification. For example, fluorescent dyes are labeled on the surface of MXenes, and the high specific surface area and good biocompatibility of MXenes are used to improve the stability and bioavailability of fluorescent dyes. MXenes itself also produces fluorescence under certain conditions and can be used directly as fluorescent probes for biological imaging. Yang et al. synthesized Nb₂C quantum dots that exhibit excellent chemical and photostable fluorescence emission [30]. These quantum dots have been successfully applied in the fluorescence sensing and imaging of heavy metal ions. Moreover, they demonstrate high biocompatibility, responsiveness to human myeloperoxidase, and unique biodegradability, ensuring their safety for *in vivo* use. Given the increasing demand for biosafety and technical stability, the Nb₂C quantum dots' combination of chemical and optical stability, biocompatibility, biodegradability, and fluorescence sensing capabilities positions them well for applications in environmental monitoring, biomedical diagnostics, visual displays, and anti-counterfeiting technologies.

5.2 Photoacoustic imaging

Photoacoustic imaging is a new imaging technique based on photoacoustic effect, which can realize high-resolution imaging of deep tissue. MXenes materials have strong absorption characteristics in the near-infrared region. When irradiated by near-infrared light, light energy is absorbed and converted into heat energy, causing thermal expansion of surrounding tissues and generating detectable ultrasonic signals. MXenes photoacoustic imaging can clearly display the location and morphology of the diseased tissue, providing important information for clinical treatment. Lu et al. employed IL stripping technology to synthesize ionic liquid (IL)-Ti₃C₂T_x MXene nanosheets that exhibit high chemical stability and show promise for applications in cancer photoacoustic imaging and combined photothermal/chemical therapy [31]. When irradiated with an 808-nm laser, these nanosheets strongly absorb near-infrared light, achieving a photothermal conversion efficiency of approximately 63.91%. As a model drug, doxorubicin (DOX) was loaded onto the IL-Ti₃C₂T_x MXene nanosheets, resulting in IL-Ti₃C₂T_x MXene@DOX nanoparticles with excellent drug loading capacity and pH/photo-sensitivity. In both *in vitro* and *in vivo* studies, IL-Ti₃C₂T_x MXene@DOX demonstrated biosafety, facilitated effective photoacoustic imaging, and successfully targeted cancer cells through a synergistic photothermal/chemotherapy approach.

Feng et al. developed a novel multifunctional two-dimensional vanadium carbide that can be selectively degraded within the tumor microenvironment (Figure 7) [32]. The V₄C₃ nanosheet demonstrates strong light absorption and photothermal conversion in the IR-II biological window. Its dual capabilities for photothermal and X-ray absorption enable both photoacoustic imaging and computed tomography (PA/CT) imaging. Additionally, the nanosheet's ability to generate ROS through photothermal

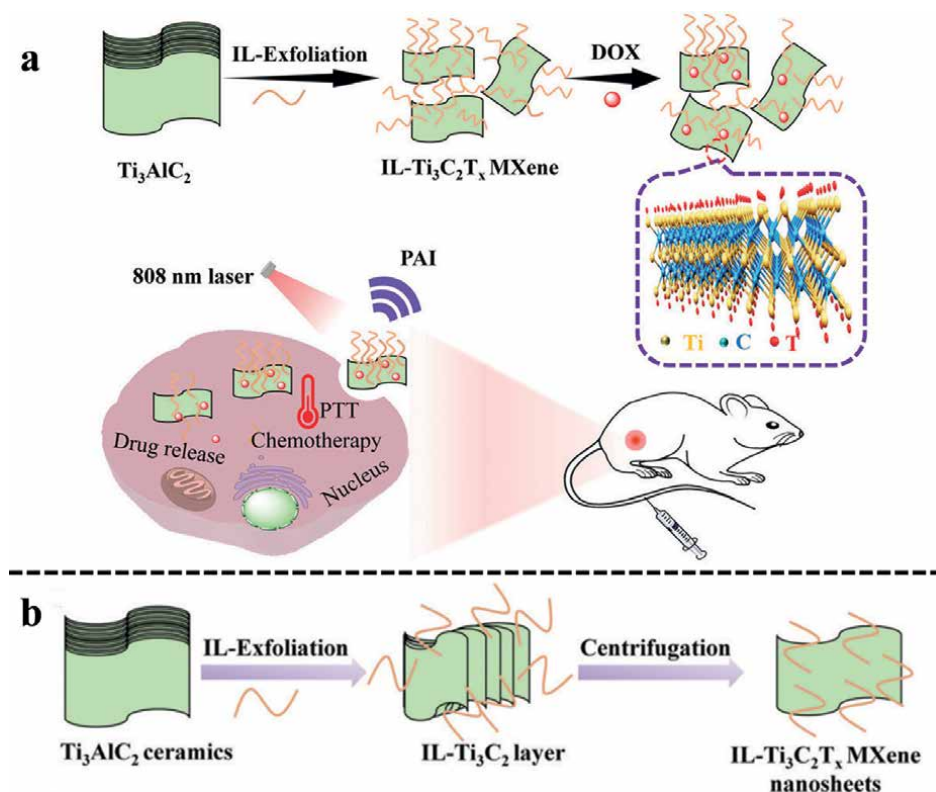


Figure 7.

(a) Preparation of Ti₃C₂T_x MXene nanosheets by IL-assisted stripping method. (b) Schematic illustration of the synthesis of IL-Ti₃C₂T_x MXene nanosheets [32].

ablation can transform cold tumors into hot tumors, inducing immunogenic cell death (ICD) and other therapeutic responses.

5.3 Magnetic resonance imaging

Magnetic resonance imaging is a widely used technique in clinic. MXenes material is paramagnetic and can be used as a contrast agent in magnetic resonance imaging. Researchers usually combine MXenes with targeted molecules to achieve targeted magnetic resonance imaging of specific tissues or cells, improving the specificity and accuracy of imaging. MXenes show great potential for medical imaging, but their application in biological imaging has been limited due to their typically diamagnetic properties. To overcome this, MXenes can be functionalized with ferromagnetic or paramagnetic compounds, as well as nanoparticles, to enhance their bioimaging capabilities. Among the different methods, covalent functionalization offers better stability for MXenes, preventing issues like self-aggregation and degradation, which are more common with electrostatic methods. For example, Neubertova et al. covalently functionalized Ti₃C₂T_x thin sheets using diethylenetriamine pentaacetic acid (DTPA) and then complexed them with Gd³⁺ ions (**Figure 8**) [33]. This modification not only enables the inherently diamagnetic Ti₃C₂T_x to exhibit a paramagnetic response for T1-MR imaging, but also helps protect the MXene surface from oxidation and improves its cytocompatibility.

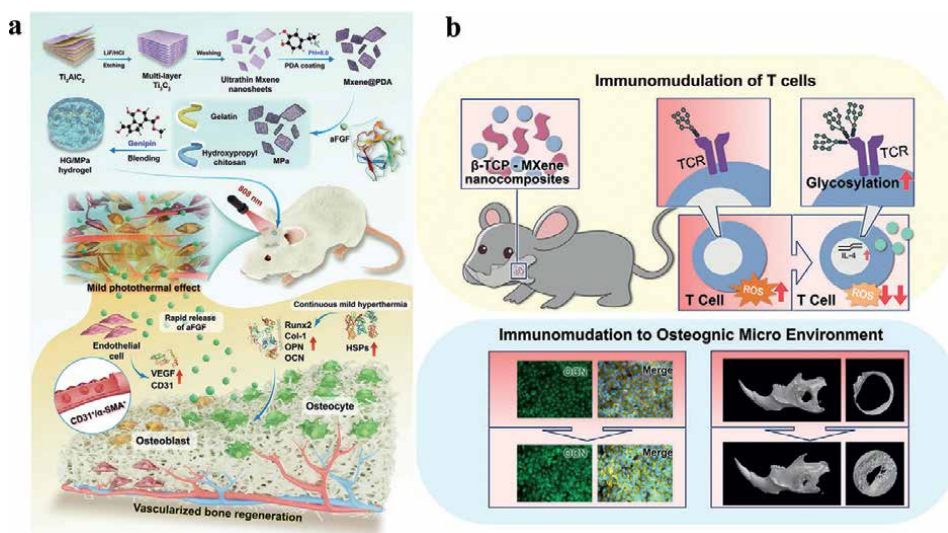


Figure 8.
 (a) A photoactivated hydrogel system (HG/MPa) with photothermal therapeutic activity and controlled drug delivery capability for regulating vascular remodeling and osteogenic differentiation. (b) Schematic diagram of T-MXene nanomaterial promoting bone formation [33].

Additionally, the chelation of Gd^{3+} prevents ion leakage, thereby broadening the potential for MXenes in clinical bioimaging applications.

MXenes materials can be combined with polymers, ceramics and other materials to prepare scaffold materials with different structures and properties to meet the needs of different tissue engineering applications. For example, the scaffold material prepared by combining MXenes material with polylactic acid (PLA) has good mechanical properties and biocompatibility, which can promote cell adhesion, proliferation, and differentiation, and has potential application value in bone tissue engineering and skin tissue engineering. Yu et al. synthesized $Ti_3C_2T_x$ MXene and incorporated β -tricalcium phosphate ceramic nanocomposite (T-MXene) to evaluate its bone induction and immunomodulatory effects [34]. The effect of T-MXene-treated T cells on bone marrow stromal cells was studied, and the therapeutic potential of bone regeneration *in vivo* was evaluated using mandibular defect model. The results showed that T-MXene increased the proportion of $IL-4^+$ T cells in primary T cells and mandibular lymph nodes, and promoted bone marrow mesenchymal stem cells and bone formation of the injured mandible. The unique function of MXene-based nanocomposites in bone immune regulation provides a basis for the exploration and application of MXene as an immune response regulator, which is expected to promote its application in regenerative medicine.

6. Application of MXenes-based materials in disease diagnosis and cancer treatment

Accurate diagnosis and effective treatment of diseases have always been central to medical research. The rapid advancement of nanotechnology has introduced novel nanomaterials, offering new possibilities for disease diagnosis and treatment. Among these, MXenes have garnered significant attention due to their excellent optical and

thermal properties, as well as their tunable surface chemistry. This has led to increasing research into their applications in biomedicine [32]. In particular, MXenes show great promise in disease diagnosis and cancer treatment. Their strong light absorption in the near-infrared region allows them to generate bright fluorescence for cancer imaging through radiative transitions, while non-radiative transitions can produce ROS for cancer therapy. Currently, the use of MXenes in cancer treatment is primarily focused on photodynamic therapy, photothermal therapy, and multimodal combination therapies [35].

6.1 Photodynamic therapy

Photodynamic therapy (PDT) utilizes photosensitizers to generate ROS under light exposure, leading to tumor cell death. Certain MXene materials have been identified as potential photosensitizers, and their combination with traditional photosensitizers may enhance therapeutic efficacy.

Zheng et al. developed a $\text{CeO}_2/\text{Ti}_3\text{C}_2$ -MXene ($\text{CeO}_2@\text{MXene}$) hybrid, where CeO_2 nanoparticles serve as a redox center [36]. These nanoparticles react with hydrogen peroxide (H_2O_2) to generate oxygen, alleviating the hypoxic tumor microenvironment and enabling type II PDT. In addition, the hybrid produces multiple ROS (e.g., superoxide and hydroxyl radicals) through type I photodynamic mechanisms. The $\text{CeO}_2@\text{MXene}$ heterojunction also exhibits nanozyme activity, enhancing the synergistic effects of type I and type II PDT for improved cancer treatment. Zhao et al. synthesized 2D Ti_3C_2 MXene nanosheets functionalized with CeO_2 nanozymes and glucose oxidase (GOD) [37]. The CeO_2 nanozymes exhibits both peroxide-like and catalase-like properties, converting H_2O_2 into hydroxyl radicals for catalytic therapy while also generating oxygen to reduce hypoxia. GOD increases H_2O_2 levels by metabolizing glucose, further disrupting the tumor's energy supply. When subjected to near-infrared laser irradiation, the Ti_3C_2 MXene facilitates both photothermal and

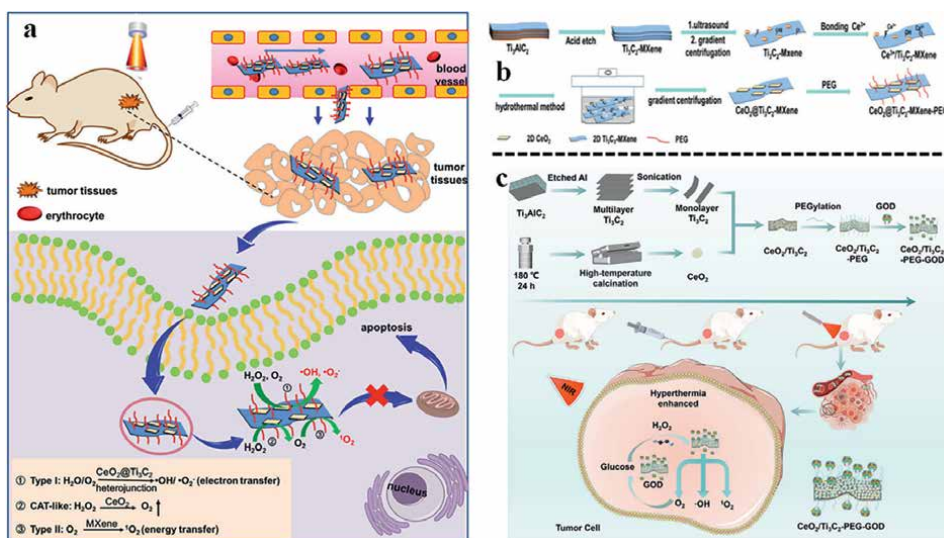


Figure 9. (a) Schematic diagram of anticancer photodynamic therapy based on the $\text{CeO}_2@\text{MXene}$ materials. (b) Schematic diagram of the composition of the $\text{CeO}_2@\text{MXene}$. (c) Preparation process of $\text{CeO}_2/\text{Ti}_3\text{C}_2$ -PEG-GOD nanomaterials and schematic diagram of anti-tumor in vivo [37].

photodynamic therapies, with thermal enhancement amplifying the catalytic effect. *In vivo* and *in vitro* studies demonstrate that the $\text{CeO}_2/\text{Ti}_3\text{C}_2\text{-PEG-GOD}$ nanocomposite exhibits strong tumor inhibition (Figure 9).

6.2 Photothermal therapy

Photothermal therapy (PTT) uses photothermal conversion materials to transform light energy into heat, raising the temperature of tumor tissue and effectively killing cancer cells. MXenes are promising materials for PTT due to their strong absorption of near-infrared (NIR) light, particularly at the 808-nm wavelength, which enables efficient tumor cell destruction. The second near-infrared region (NIR-II) offers deeper tissue penetration, making it ideal for targeting tumors located deeper in the body. However, the search for optimal photothermal agents (PTAs) has been hindered by challenges in dose selection.

Tang et al. explored the potential of anionic solid-solution MXenes as PTAs. These materials, with their diverse chemical composition and tunable photoresponse, exhibit enhanced NIR-II absorption due to the regulation of free carrier density *via* anion modification [38]. Specifically, $\text{Ti}_3\text{C}_{1.23}\text{N}_{0.77}$ with its high nitrogen content, demonstrated an extinction coefficient of $43.5 \text{ L g}^{-1} \text{ cm}^{-1}$, and *in vivo* experiments confirmed the effectiveness of photothermal tumor treatment.

6.3 Multimodal combination therapy

MXenes also show versatility in combining multiple therapeutic modalities. For instance, V_4C_3 nanoplates exhibit both excellent photothermal and X-ray absorption properties, enabling dual-mode photoacoustic imaging and computed tomography (CT) imaging. Additionally, these nanoplates can convert cold tumors into hot tumors through photothermal ablation and ROS generation, inducing immunogenic cell death. This synergy of imaging and treatment enhances the overall effectiveness of cancer therapy.

Liang et al. developed nanoclusters ($\text{RhRu}/\text{Ti}_3\text{C}_2\text{T}_x$) by incorporating a RhRu alloy into 2D titanium carbide, which enables chemokinetic, photodynamic, and photothermal treatments of osteosarcoma [39]. These nanoclusters, with an average size of 3.6 nm and uniform distribution, exhibit excellent catalase- and peroxidase-like activities. Theoretical calculations reveal significant electron transfer between RhRu and $\text{Ti}_3\text{C}_2\text{T}_x$, enhancing H_2O_2 adsorption and boosting enzyme-like activity. The $\text{RhRu}/\text{Ti}_3\text{C}_2\text{T}_x$ nanoenzyme not only serves as a photothermal agent to generate heat but also acts as a photosensitizer, catalyzing the conversion of O_2 into singlet oxygen ($^1\text{O}_2$). Its combined chemokinetic, photodynamic, and photothermal therapeutic effects on osteosarcoma have been validated both *in vitro* and *in vivo*.

7. Challenges and future perspectives

Despite the promising potential of MXenes in biomedicine, several challenges remain before their widespread clinical application. First, the synthesis and reproducibility of MXenes pose significant obstacles, particularly when considering mass production for biomedical use. Second, the potential toxicity of MXenes, especially at high doses or with long-term exposure, remains a concern. While some studies suggest that MXenes exhibit low toxicity and are biocompatible, the long-term health

effects are not yet fully understood, necessitating further research to evaluate their safety. Lastly, to achieve specific biomedical functions, precise surface functionalization of MXenes is required. However, ensuring the stability of these functionalized materials in the biological microenvironment presents an additional challenge.

Currently, MXene materials are diversifying, with a growing number of low-toxicity, biocompatible variants being used in clinical settings. Functionalized MXenes continue to play a significant role in clinical diagnostics and treatment. Looking ahead, these materials hold promise for applications in immunotherapy, where they could regulate immune responses, complement other treatment modalities, and contribute to the ongoing advancement of human medicine.

8. Conclusion

MXene materials have demonstrated significant potential in biomedical engineering, with notable advancements in areas such as drug delivery, biosensing, antibacterial applications, tissue engineering, bioimaging, and disease diagnosis and treatment. However, several challenges remain in their practical application. Future research should focus on assessing their biosafety, developing simpler and more efficient surface modification techniques, and addressing issues related to large-scale production and cost. As research progresses and technology advances, MXenes are poised to make substantial breakthroughs in biomedical engineering, contributing meaningfully to human health.

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Conflict of interest

The authors declare no conflict of interest.

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Solution-Processed $\text{Ti}_3\text{C}_2\text{T}_x$ MXene Thin-Films: Conductivity Trends and Charge Transport Mechanisms

Jurij Urbančič

Abstract

Progress in the field of MXenes relies on a thorough understanding of how synthesis processes impact their performance and the ability to achieve consistent reproducibility of results. This review provides an overview of titanium carbide ($\text{Ti}_3\text{C}_2\text{T}_x$) MXene, focusing on its electrical conductivity when utilized in the fabrication of thin films from solution. We discuss the relationship between conductivity and film thickness, as well as the underlying charge transport mechanisms, highlighting its dual nature characterized by band-like conduction within individual flakes and thermally activated hopping between flakes. Additionally, the evolution of electrical conductivity, spanning from 10^2 to 10^4 S/cm, is discussed in relation to synthesis techniques, flake quality, and surface terminations. The findings underscore the significance of structural and morphological optimization in achieving high-performance MXene films.

Keywords: Ti_3C_2 , MXenes, 2D materials, thin films, conductivity, charge transport, hopping, mobility

1. Introduction

MXenes are a family of two-dimensional (2D) materials derived from a layered metallic ceramic known as the $\text{M}_{n+1}\text{AX}_n$ phase (where $n = 1, 2$, or 3), or in short, just MAX. In this structure, M represents a transition metal, A is an element from group IIIA or IVA, and X is carbon and/or nitrogen. The selective removal of A-layer atoms results in the formation of $\text{M}_{n+1}\text{XT}_x$, a class of materials now widely known as MXenes. Here, T_x denotes surface termination groups that are determined by the synthesis and delamination processes. Among the MXenes, $\text{Ti}_3\text{C}_2\text{T}_x$ synthesized from the Ti_3AlC_2 MAX phase was the first to be discovered [1] and remains the most widely studied due to its unique metallic and hydrophilic behavior.

Moreover, the ability to fabricate conductive films with controllable thicknesses presents exciting opportunities for various applications, as thin films stand out as a promising avenue for high-performance electronic applications due to the combination of conductivity and transparency [2, 3]. One notable use is as transparent and conductive electrodes on flexible substrates, which are crucial components in modern

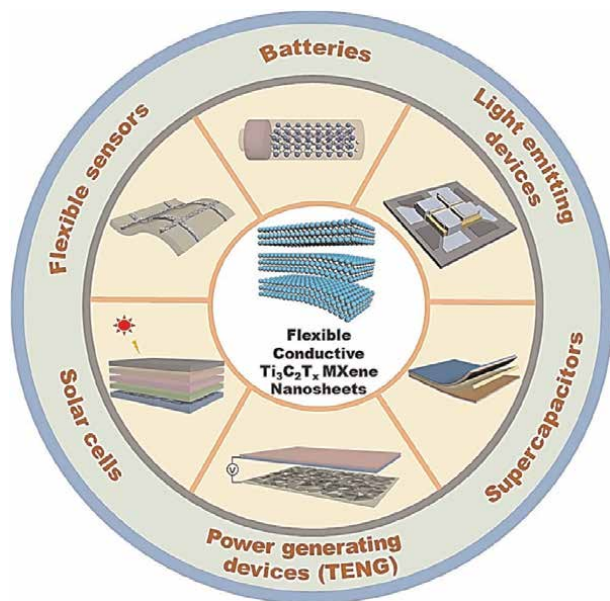


Figure 1.

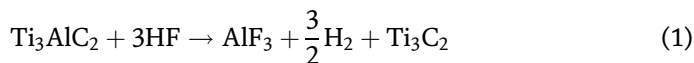
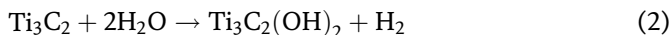
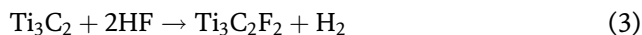
Novel uses of Ti_3C_2 -based MXene flakes (nanosheets) as versatile and flexible conductive electrodes in modern electronic devices. Illustration provided with permission from Meena et al. [4].

electronics, such as photovoltaic cells, displays, sensors, and electromagnetic interference shielding devices. Therefore, the main applications of Ti_3C_2 MXene are schematically highlighted in **Figure 1** [4].

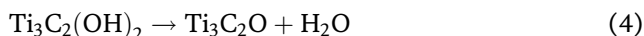
In this review, we explore the nature of charge transport in thin films made of $\text{Ti}_3\text{C}_2\text{T}_x$ flakes deposited from solution. Unlike epitaxial grown MXene films [3], which benefit from highly ordered crystalline growth, solution-processed films are typically composed of percolated networks of flakes. These networks introduce additional complexities, such as inter-flake junction resistance and structural inhomogeneities, which significantly influence macroscopic charge transport. By focusing on solution-processed films, this chapter addresses the practical challenges associated with real-world applications, where scalable and cost-effective fabrication methods are critical. The observed trends in reported charge carrier conductivity reveal an improvement over time, alongside a better understanding of the charge carrier mechanism on the macroscopic level. These results reinforce the critical role of structural optimization in determining MXene conductivity. The substantial increase in conductivity over time demonstrates the rapid progress in MXene research, setting a strong foundation for future developments.

2. MXene thin film fabrication

The $\text{Ti}_3\text{C}_2\text{T}_x$ synthesis typically involves the chemical etching of the aluminum (Al) atoms from the MAX structure, which can be achieved using various chemical approaches. In the most straightforward approach, fluoride-based acids or salts (like HF, LiF/HCl) are used, resulting in -F, -OH, and = O termination [5]. The resulting surface terminations, -F and -OH, are a result of the etching process, as described by the following simplified reactions [6]:



Surface termination additionally includes = O [7–9], which has been explained as resulting from an equilibrium-driven reaction where surface-bound OH groups recombine to form H_2O and O:



MXenes are likely to stay fully terminated, indicating strong bonding between the Ti and T_x . After the selective removal of Al atoms, the layered MXene structure can be expanded by intercalating large organic molecules, such as dimethyl sulfoxide (DMSO) [8]. This process weakens the interlayer interactions, facilitating the separation of individual layers during ultrasonication, thus producing flakes similar to graphene and other 2D materials [10]. These flakes can then be dispersed in aqueous and organic solutions after the delamination [8, 10]. The schematic view of this process is further illustrated in **Figure 2a** [11].

The quality of the delamination process and flake quality can be verified using the atomic force microscope (AFM), as shown in **Figure 2b**, with the expected single flake height of around 1.5 nm [12]. Once the MXene flakes are prepared and dispersed

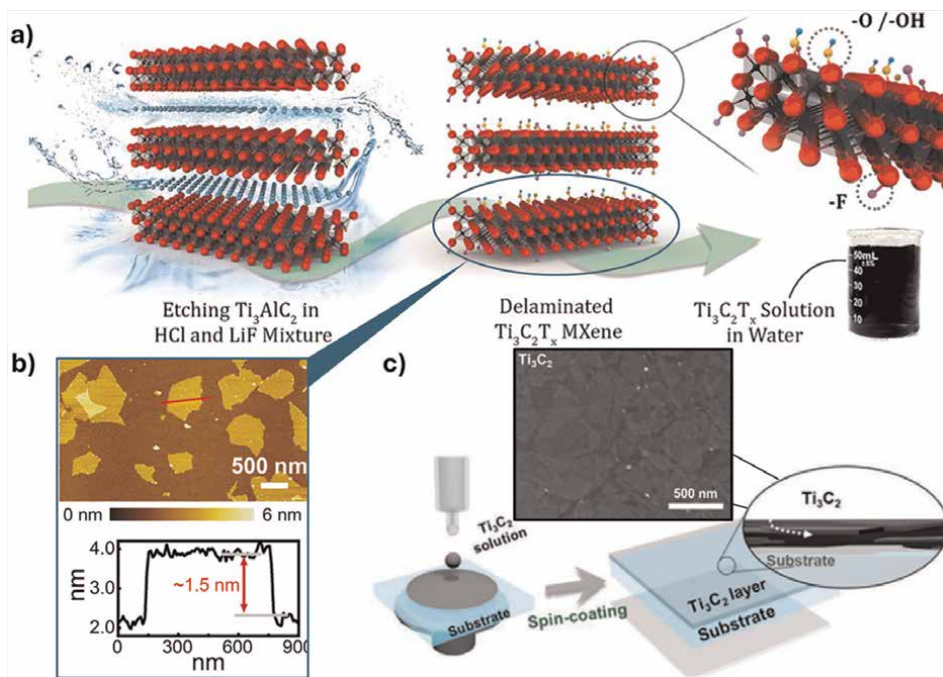


Figure 2. (a) Schematic view of solution preparation containing dispersed $\text{Ti}_3\text{C}_2\text{T}_x$ MXene flakes, reprinted with permission from Vahid Mohammadi et al. [11]. (b) AFM image of MXene flakes deposited from the solution and the corresponding height profile of a single flake. Image courtesy of Bai et al. [12]. (c) Illustration of a $\text{Ti}_3\text{C}_2\text{T}_x$ thin film preparation via spin-coating on a flexible substrate with the corresponding scanning electron microscope (SEM) image of the surface. Adapted with permission from Ahn et al. [13].

in a stable colloidal solution, thin films can be fabricated from the resulting solution using various deposition techniques, such as spin- or dip-coating [13, 14], rolling [15], spray-coating [16, 17], and vacuum filtration [18]. These methods are particularly advantageous due to their simplicity, scalability, and ability to produce films with thickness control. For instance, **Figure 2c** illustrates an MXene film prepared *via* spin-coating, and the overlap of the flakes was inspected using the scanning electron microscope (SEM) [13].

3. Electronic properties of MXene thin films

Ti_3C_2 , like most MXenes, exhibits metallic conductivity (σ) due to its unique layered structure and the presence of delocalized electrons [19], resulting in the valance and conduction band overlap at the Fermi level, as shown in **Figure 3a** for its density of states (DOS) [20]. In general, MXene solution-processed thin films consist of a network of single-layered flakes deposited on a substrate. These flakes form a network of percolated structures with varying degrees of ordered alignment. Hence, the conductivity can be described using a model of 2D conductive nanosheets connected in a percolated network [21, 22]. The flakes are interconnected *via* junctions where neighboring flakes are separated by a narrow van der Waals gap. This arrangement plays a critical role in determining the overall electrical properties of the thin film. Importantly, electrical conductivity across the thin film is not solely dependent on the intrinsic properties of individual MXene flakes but is also constrained by the movement of charge carriers across these inter-flake junctions.

To explain this transport, the overall network can be viewed as consisting of multiple well-defined conductive paths in parallel. Within an individual current path

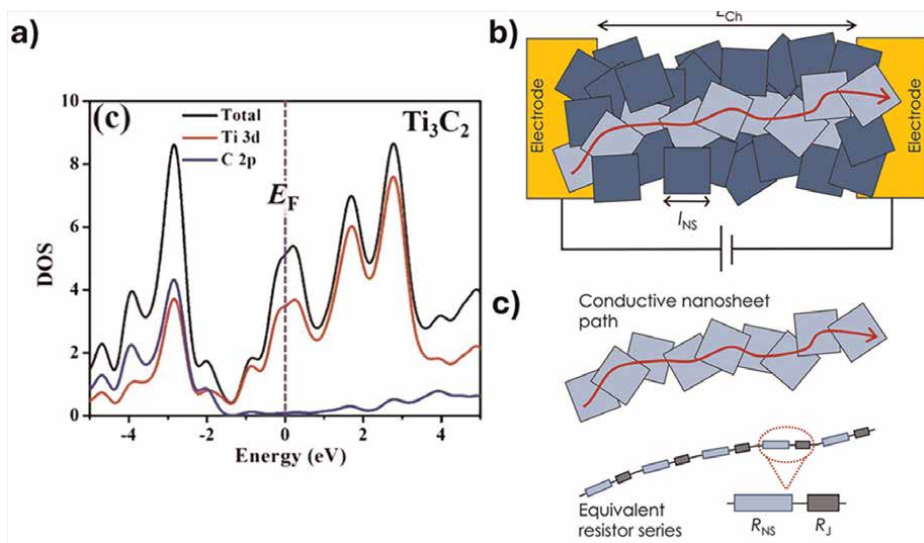


Figure 3.

(a) Density of states (DOS) plot for Ti_3C_2 MXene. Figure taken with permission from Low et al. [20]. (b) Schematic illustration of a single conducting path consisting of a linear array of flakes. (c) This conducting path can be considered as a chain of resistor pairs, with each pair consisting of a resistance representing a nanosheet (R_{NS}) and one representing the inter-sheet junction (R_J). Both (b) and (c) images are reproduced with permission from Gabbett et al. [21].

(**Figure 3b**), charge carriers traverse a linear array of nanosheets (MXene flakes in our case), crossing an inter-particle junction each time they move between adjacent sheets. This arrangement can be modeled as a linear array of flake-junction pairs, where each pair is described by two resistors representing the average nanosheet resistance (R_{NS}) and junction resistance (R_j), as shown in **Figure 3c**. Therefore, the conductivity of this network can be expressed as [21]:

$$\sigma_{Net} \propto \frac{1}{\left[1 + \frac{R_j}{R_{NS}}\right] \left[1 + \frac{1}{A_{NS}d_{NS}}\right]} \quad (5)$$

where A_{NS} is the nanosheet cross-sectional area and d_{NS} is the average distance the charge travels through a nanosheet.

In more than a decade of research, various electrical conductivities have been reported for MXene thin films, ranging from single-flake measurements to film thicknesses of several micrometers. These results are presented in **Figure 4** and show a conductivity spanning from 10^2 S/cm to 10^4 S/cm range [13, 14, 23–40], with the highest reported value being 2.4×10^4 [36], highlighting the variability in electrical performance. The electrical conductivity of MXene films fluctuates significantly across these studies, reflecting the influence of synthesis methods and structural properties.

Another important observation from the data is the dependence of conductivity on film thickness. References that report conductivity for MXene films of varying thicknesses [13, 26–28, 33] consistently show a decrease in conductivity with increasing thickness. Single-flake conductivities are also included for comparison, demonstrating the intrinsic properties of individual flakes. The dependence of conductivity on thickness is likely attributed to the cumulative effect of these inter-flake junctions in

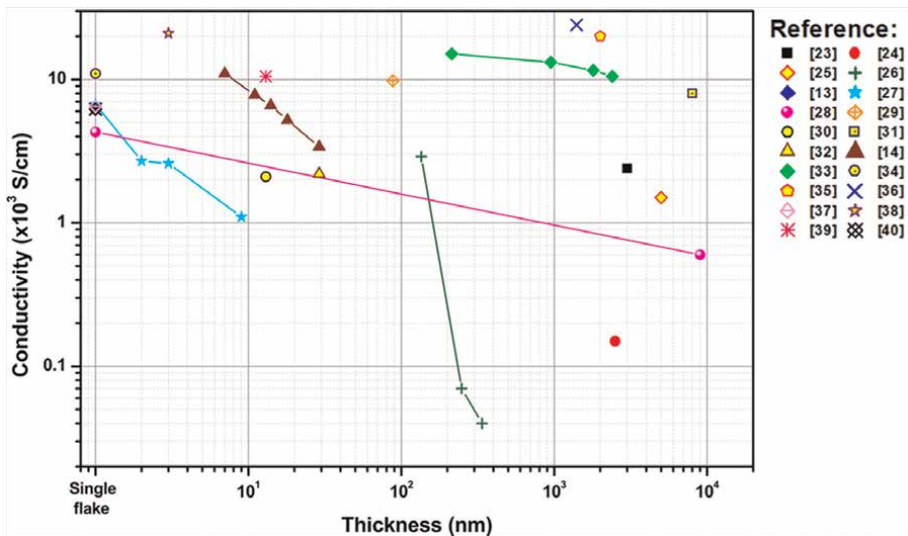


Figure 4. Reported conductivity as a function of MXene film thickness from various references. The plot also highlights the relationship between film thickness and conductivity, showing that thinner films generally exhibit higher conductivity. The different markers represent data from specific studies (referenced in the legend), illustrating variability due to differences in synthesis methods, flake quality, and deposition techniques.

thicker films. As the thickness increases, the number of flakes and junctions within the network also increases, introducing additional parasitic junction resistances (R_j) that can significantly exceed the intrinsic resistance of individual flakes (R_{NS}) [41]. While R_{NS} is an intrinsic material property, R_j is highly dependent on the thin film morphology [42]. In thicker films, the misalignment and stacking disorder of MXene flakes amplify these parasitic effects, further hindering charge transport. Thus, a good in-plane alignment of MXene flakes in thinner films enhances conductivity by minimizing the number of junctions and optimizing charge transport pathways, whereas thicker films suffer from increased junction resistance, leading to reduced conductivity.

4. Charge carrier transport mechanism

Theoretical studies [43–45] of MXenes predict a band-like transport mechanism, which has been experimentally confirmed through temperature-dependent electric resistivity measurements on a single flake, as shown in **Figure 5a** [40]. These

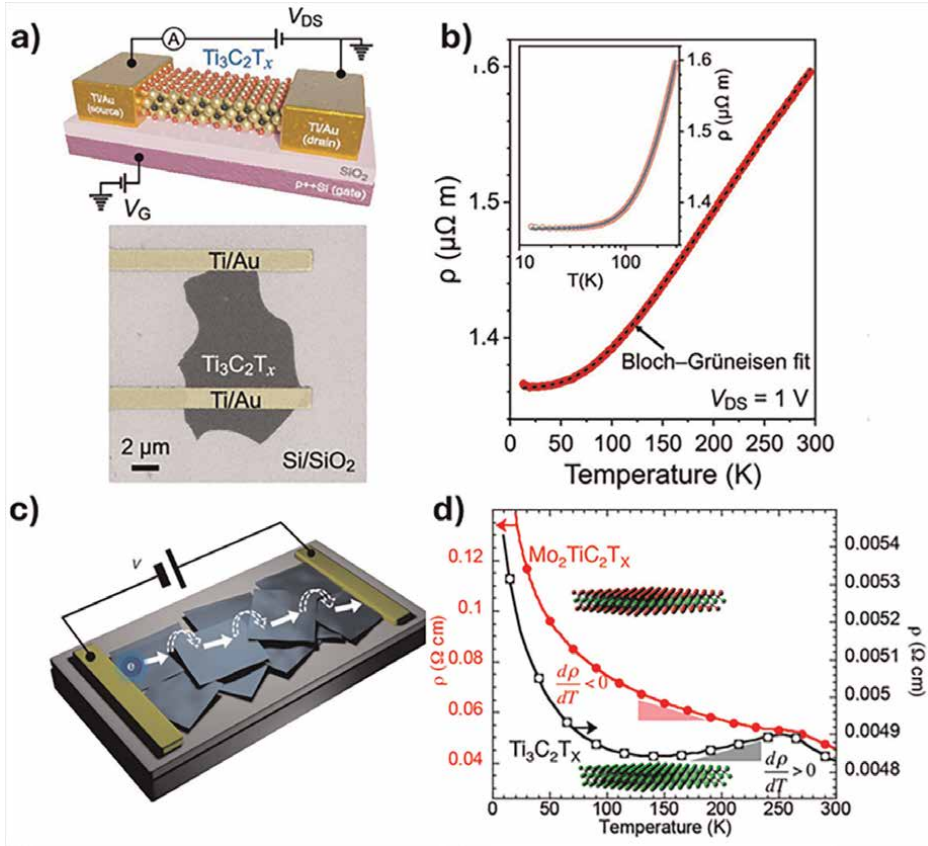


Figure 5. (a) Schematic of an FET with a MXene flake as the channel. (b) Corresponding temperature-dependent resistivity showing an increase with temperature (band-like transport). (c) Schematic of hopping conduction in MXene thin films. (d) Examples of MXene thin films exhibiting a decrease in resistivity with increasing temperature (hopping-like transport). Images (a) and (b) are taken from Lipatov et al. [40], image (c) from Zheng et al. [46], while image (d) is from Anasori et al. [47].

measurements reveal that resistivity increases with temperature (**Figure 5b**), a characteristic feature of band-like conduction caused by phonon scattering.

In contrast, temperature-dependent resistivity measurements of MXene thin films suggest that hopping conduction is the dominant transport mechanism, as schematically illustrated in **Figure 5c** [46]. Experimental data (**Figure 5d**) show a decrease in resistivity with increasing temperature for $\text{Ti}_3\text{C}_2\text{T}_x$ and $\text{Mo}_2\text{TiC}_2\text{T}_x$ MXenes [47]. This behavior indicates a thermally activated hopping process, where charge carriers move between localized states created by inter-flake junctions or structural disorder. Such behavior aligns with the characteristics of solution-processed MXene films, where inter-flake resistance plays a significant role in charge transport. Similar trends have been observed across other MXenes, highlighting this as a common characteristic of the material family [48–50].

A unifying mechanism to address this discrepancy was presented in Zheng et al. [46]. In this picture, inside the single flake, the band-like transport is dominating, while between flakes, the transport occurs *via* thermally activated hopping. Using optical-pump terahertz-probe (OPTH) spectroscopy, the transport properties of charge carriers were probed in a contact-free, non-invasive manner. This approach allowed for the characterization of short-range transport [51, 52]. In this experiment, illustrated in **Figure 6a**, the optical excitation results in heating up the electron gas and the probe terahertz pulse probes the photoconductivity. Such a method proves highly effective for analyzing short-range transport within individual flakes, as the picosecond duration of the terahertz pulse drives the charge carrier over a distance of only a few tens of nanometers, that is, within the flake.

The transient negative change photoconductivity ($\Delta\sigma_{\text{opt}}$) measured for Ti_3C_2 in **Figure 6b** is due to the heating of the lattice due to the photoexcited hot carriers heating the lattice and the resulting enhancement of carrier scattering with phonons. As the lattice gradually cools over hundreds of picoseconds, transferring heat to the substrate and the unexcited regions of the film, the conductivity of the MXene film recovers [53]. Measurements at different pump fluences further confirm this behavior, with higher fluences resulting in a larger negative $\Delta\sigma_{\text{opt}}$. This response underscores the metallic nature of the material, dominated by band transport.

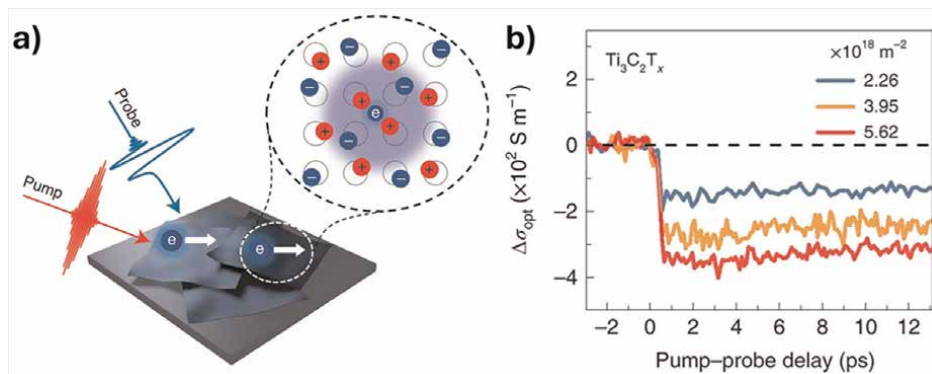


Figure 6.
 (a) Ultrafast optical-pump terahertz-probe (OPTH) experiment and (b) the fluence-dependent, time-resolved photoconductivity on $\text{Ti}_3\text{C}_2\text{T}_x$ thin films, following photoexcitation using 1.55 eV pump. Images courtesy of Zheng et al. [46], used with permission.

As already stated, transport across the whole thin film (long-range macroscopic level) was shown to be dominated by hopping. Besides the static electrical measurements, this was also confirmed in the time-of-flight photoconductivity (TOFP) investigation of 12 nm thick $\text{Ti}_3\text{C}_2\text{T}_x$ thin film deposited on a quartz substrate [54]. In the TOFP method [55], a constant bias voltage, V_b , is applied between two electrodes deposited on the active layer, and a laser is focused near one electrode. What is followed is the laser excitation of charge carriers that are drifting toward the other electrode under the influence of V_b , resulting in a decreasing transient current $I(t)$.

Figure 7a shows a $I(t)$ for different values of V_b . When the charge carrier reaches the electrode, a characteristic change of slope is observed in the transient time t_{tr} , from which the mobility (μ) can be calculated using the relation [56].

$$\mu \propto \frac{1}{V_b t_{tr}} \quad (6)$$

The charge carrier mobility which reflects how efficiently charge carriers can traverse the material under an applied electric field. Mobility is also directly related to electrical conductivity (σ) through the equation $\mu = nq$, where n is the charge carrier concentration and q is the elementary charge [57].

The resulting extracted values of μ and t_{tr} are presented in **Figure 6b**, and it shows mobility dependence on the V_b , going from $146 \text{ cm}^2/\text{Vs}$ at -50 V to $279 \text{ cm}^2/\text{Vs}$ at -150 V . The dependence on the electric field is a characteristic of disordered systems, where hopping is the prevalent mechanism, arising from the lowering of the Coulomb energy barrier between the energy states by the applied electric field (Poole-Frenkel effect [58–60]). On the other hand, the relatively high carrier mobility is like in crystalline systems with band transport. This behavior is consistent with a dual-type transport mechanism, where contributions from both hopping and band-like transport coexist, highlighting the complex nature of the charge carrier dynamics in the system.

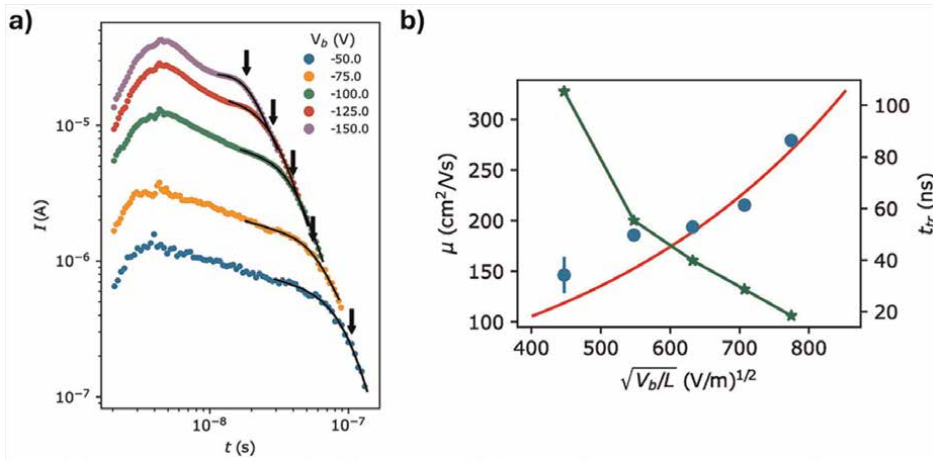


Figure 7. (a) Time-dependent photocurrent $I(t)$, measured on a 12 nm thick $\text{Ti}_3\text{C}_2\text{T}_x$ film deposited on a quartz substrate. Different colors represent measurements performed at values of the bias voltage V_b . The arrows indicate the transit time t_{tr} , when the electrons arrive across the channel length. (b) The t_{tr} (green stars) and the electron mobility (blue circle) as a function of the square root of the V_b . The red solid line represents a fit using the Poole-Frenkel equation. Images reproduced with permission from Urbančič et al. [54].

5. Conductivity trends and influencing factors in MXene thin films

Over the years, a clear trend of improvement in conductivity has emerged, as illustrated in **Figure 8**, which presents a collection of measured conductivities over time. Early works reported relatively modest conductivities, but subsequent studies have demonstrated significant advancements in film preparation techniques, leading to marked improvements in charge transport properties. The linear fit of the data and the accompanying box plot highlight a gradual and consistent increase in conductivity, reflecting the progressive optimization of synthesis and fabrication methods. Ti_3C_2 thin films with conductivities in the range of 10^4 S/cm now rival the performance of graphene films [61].

This improvement can be attributed to the optimization of synthesis processes resulting in high-quality MXene flakes with increased flake size [33] and the reduction of atomic defects present [27], like missing Ti atoms (Ti vacancies) [62]. Generally, the employment of an in situ HF formation yields better flake quality results [36]. In a film, large particle size translates into a large cross-sectional area A_{NS} , resulting in a conductive path with fewer junctions between flakes. Regarding the film layer fabrication, the well alignment of flakes reduces their jamming and non-parallel configuration, therefore also decreasing the parasitic junction resistance R_j . Both factors influence the overall conductivity, as indicated in Eq. 5 and also experimentally corroborated [63]. Thus, the improved MXene exfoliation and deposition methods resulting in a good inter-flake connectivity also enhance the charge transfer inside the film. An average size of flakes around 5 μm indicates high-quality synthesis; the flake orientation with the (002) plane parallel to the substrate yields smooth conductivity through the film [54].

Another important issue is the surface termination. Density functional theory (DFT) predicted that surface functionalization reduces the DOS at the Fermi level, resulting in a decrease of overall conductivity via the reduction of the number of charge carriers [64–66]. This was experimentally confirmed with the removal of -OH,

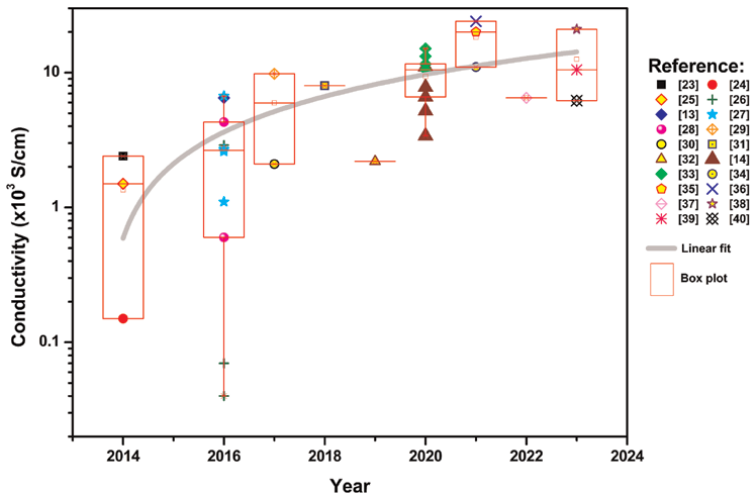


Figure 8. Reported conductivities of MXene thin films from 2014 to 2023. The red boxes represent the box plots of the data, highlighting the variability and range of reported values, while the gray line indicates the linear fit, illustrating a clear trend of increasing average conductivity over time as synthesis and fabrication methods improved.

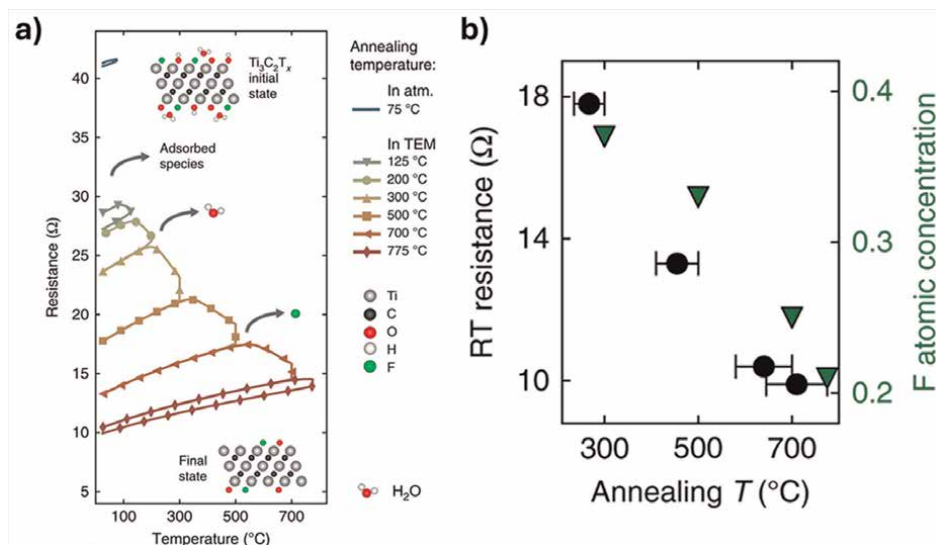


Figure 9. (a) $\text{Ti}_3\text{C}_2\text{T}_x$ electronic resistance evolution vs. temperature measurements, performed at various annealing temperatures in a TEM. (b) $\text{Ti}_3\text{C}_2\text{T}_x$ post-annealing resistance measurement at room temperature (black circles) and the resulting -F concentration (green triangles). Republished with consent from Hart et al. [67].

-F, and = O termination species through high-temperature annealing and the resulting increase in sample conductivity [67]. In this experiment, the temperature-dependent resistance was measured at various temperatures *in situ* inside a transmission electron microscope (TEM), shown in **Figure 9a**. The de-functionalization of -OH happens at temperatures around 375 $^{\circ}\text{C}$, where it is either removed or converted to a more stable = O termination. Temperatures from 400 to 775 $^{\circ}\text{C}$ result in the loss of -F terminations. Post-annealing resistance measurements at room temperature (**Figure 9b**) also confirm the correlation between the annealing temperature, -F termination, and the resulting conductivity. These findings illustrate that the measured conductivity of MXenes is significantly influenced by the type and amount of surface terminations present.

Understanding and controlling surface termination levels provide new opportunities to enhance the performance of MXene-based applications, including electromagnetic interference shielding and optoelectronics. However, optimizing surface termination alone is not sufficient, as the material's interaction with environmental factors can introduce additional challenges. For instance, exposure to oxygen and water results in the formation of titanium dioxide (TiO_2) [68] that adversely affects the electrical properties [69]. Therefore, drying at elevated temperatures can remove interlayer water from MXene films, enhance their conductivity, and provide environmental stability [70].

6. Conclusion and outlook

This review highlights the significant advancements in understanding and optimizing the electrical conductivity of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene thin films. Over the years, improvements in synthesis techniques, flake alignment, and surface termination have substantially enhanced charge transport properties. The dual transport mechanism

—band-like conduction within individual flakes and thermally activated hopping between flakes—provides a comprehensive framework for explaining conductivity trends in MXenes. The observed trends reinforce the critical role of structural optimization in determining MXene conductivity. Ultrathin films remain a promising avenue for high-performance electronic applications, while thicker films could benefit from advancements in interlayer alignment and defect engineering. The substantial increase in conductivity over time demonstrates the rapid progress in MXene research, setting a strong foundation for future developments in energy storage, flexible electronics, and sensors.

Looking ahead, further progress in MXene research will likely depend on overcoming key challenges, including controlling environmental stability, minimizing inter-flake resistance, and scaling up synthesis methods for industrial applications. Addressing these issues could unlock new potential for MXenes in next-generation technologies, including flexible electronics and advanced sensors. Continued collaboration between theoretical modeling and experimental validation will be essential to fully realize the potential of $Ti_3C_2T_x$ and related MXene materials.

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Conflict of interest

The authors declare no conflict of interest.

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Tailored Terminal Groups in MXenes for Fast-Charging and Safe Energy Storage

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Abstract

The development of metal-ion batteries (MIBs) necessitates advanced thermal management strategies to prevent thermal runaway and ensure safe operation during rapid charging and discharging, particularly under elevated temperatures. While traditional thermal management approaches focus predominantly on optimizing separators and electrolytes, innovative electrode materials can significantly enhance these efforts. This chapter explores the potential of surface-terminated MXenes with exceptional electrical conductivity and low infrared emissivity to improve thermal regulation in MIBs. Recent advances in one-step organic Lewis acid-assisted gas-phase reaction complemented by vacuum filtration to prepare a variety of tailored MXenes have been developed to integrate high-rate capacity with reduced heat generation during ion storage. Typically, Se-terminated Nb_2CSe_2 demonstrates a remarkable 1.5-fold enhancement in Li^+ -storage capacity, achieving $\sim 220 \text{ mAh}\cdot\text{g}^{-1}$ at a current density of $1 \text{ A}\cdot\text{g}^{-1}$ by the fifth cycle. This performance improvement stems from superior electrical conductivity, structural stability, and high mid-infrared permittivity, which contribute to minimized thermal radiation. Additionally, computational analyses highlight that the alignment of enhanced permittivity and conductivity along the z-direction significantly reduces heat radiation from these electrodes. This chapter underscores the potential of tailored terminal groups in various MXenes, emphasizing how engineered surface functionalities can lead to the development of flexible electrodes with intrinsic self-thermal management capabilities for the safe and efficient energy storage of fast-charging MIBs. The insights provided herein illuminate the role of surface-terminated 2D materials in advancing the performance and safety of next-generation energy storage technologies.

Keywords: thermal management, surface-terminated MXenes, electrical conductivity, infrared emissivity, energy storage

1. Introduction

Metal-ion batteries (MIBs), including lithium-ion (LIB), sodium-ion (NIB), and potassium-ion batteries (PIB), have become essential energy sources for electric

vehicles, portable electronics, and various modern applications [1–4]. Effective thermal management is critical to ensuring optimal performance and safety, particularly under high-rate charging conditions. Managing heat generation and enhancing heat dissipation within electrode materials and electrolyte interfaces are crucial for achieving reliable operation of high-energy metal-ion batteries [5–7]. Current research has predominantly focused on improving thermal properties through innovations in separators [8, 9] and electrolytes [10–12], yet significant heat generation typically arises from charge transfer processes within the electrode during cycling [13].

To mitigate temperature increases and enhance the stability and safety of metal-ion batteries, it is important to design electrodes with improved thermal properties. Despite advancements in modifying materials to sustain electrochemical performance at elevated temperatures [14–16], there remains a critical need for electrode materials that exhibit advanced self-thermal management (STM) capabilities to effectively reduce both heat generation and thermal radiation for commercial applications.

Theoretical analyses indicate that the heat generated by electrode materials during (dis)charging is closely linked to their conductivity and resistance, both of which increase with current density and voltage. However, effective heat transfer is often limited by the high mid-infrared (IR) emissivity of these materials [17–22]. An ideal STM electrode should possess low resistance and high electronic conductivity to minimize heat generation, while also demonstrating low mid-IR emissivity in the 2.5–20 μm range to facilitate heat reflection or transmission [20, 23]. Although many inorganic materials have excellent conductivity, they often fail to meet the low mid-IR emissivity requirements necessary for effective thermal management in battery applications [24].

Among emerging candidates, MXenes—2D transition metal carbides and nitrides characterized by the formula $\text{M}^{n+}_1\text{X}_n\text{T}_x$, where M represents transition metals, T_x denotes surface terminal groups, and X typically refers to carbon or nitrogen—have attracted significant attention due to their remarkable electronic, optical, and thermal properties [25–29]. The tunability of MXenes' surface chemistries allows for the modulation of their electronic characteristics, facilitating phenomena such as metal-to-insulator transitions and superconductivity [30–37]. Notably, various MXenes, such as titanium carbide ($\text{Ti}_3\text{C}_2\text{T}_x$), niobium carbide (Nb_2CT_x), zirconium carbide (Zr_2CT_x), and hafnium carbide (Hf_2CT_x), exhibit superior electrical conductivity and stability, making them suitable for high-rate energy storage applications [38–45].

Despite these advantages, conventional synthesis methods for MXenes, which rely on selectively etching A-group elements from precursor MAX phases, often lead to limitations, including lower specific capacities for lithium and other metal ion storage, suboptimal electronic conductivity, residual impurities, and poor structural stability due to disordered surface terminations ($-\text{O}$, $-\text{OH}$, $-\text{F}$) [46–50]. Therefore, developing straightforward methods for producing MXenes with specific surface terminal groups that can synergistically enhance thermal management while maintaining high-rate and energy storage capabilities remains a significant challenge.

In this context, this chapter introduces the one-step sustainable method for the large-scale production of ordered S/Se-terminated MXenes. This approach employs the synergistic dehalogenation of hexachlorobenzene combined with solid-state conversion, streamlining traditional processes and eliminating the need for additional etching or complex functionalization steps [51–55]. The typical Se-terminated Nb_2CSe_2 showcases impressive properties, including a carrier concentration of approximately $1.9 \times 10^{21} \text{ cm}^{-3}$ and superior electronic conductivity ($\sim 7.1 \times 10^4 \text{ S}\cdot\text{m}^{-1}$), nearly 2000 times that of disordered Nb_2CT_x . Furthermore, Nb_2CSe_2 flexible, free-standing

films prepared by vacuum filtration display low mid-IR emissivity, enhancing thermal management during cycling, particularly under high-rate and temperature conditions. This chapter highlights the potential of tailored terminal groups in various MXenes to enhance the performance of MIBs, paving the way for the development of flexible, safe batteries that offer rapid charging and high energy capabilities across a range of applications.

2. Mechanism of tailored terminal groups in MXenes for fast-charging applications

The increasing demand for electric vehicles and fast-charging technologies underscores the necessity of developing electrode materials capable of efficiently delivering energy while maintaining safety [5–7]. Fast-charging batteries should not only achieve high capacities but also manage thermal properties effectively to prevent issues such as dendrite formation and thermal runaway. The exploration of tailored terminal groups in MXenes presents a novel strategy to enhance overall performance, enabling faster charging rates while ensuring stability and safety. Two-dimensional (2D) transition metal carbides and/or nitrides, collectively known as MXenes ($M^{n+}_1X_nT_x$; $M = \text{Ti, V, Nb, Ta}$; $X = \text{C, N}$), have emerged as promising candidates in the realm of fast-charging batteries due to their tunable electronic properties and rich surface chemistry [25–27, 56, 57]. Their exceptional conductivity, combined with a large surface area, positions MXenes as favorable materials for energy storage and conversion applications [30–33, 38–43, 58–63]. However, several challenges impede their broader integration into commercial battery systems.

Traditional methods for synthesizing MXenes typically involve the selective etching of precursor MAX phases, which can be complex and often utilize hazardous chemicals [46–48]. Moreover, MXenes produced via conventional acid etching are frequently terminated with disorganized functional groups ($-\text{O}$, $-\text{OH}$, $-\text{F}$, $-\text{Cl}$), which can severely limit their electronic conductivity and chemical stability [49, 50, 64]. These disordered terminal groups also restrict the specific capacity of MXenes, typically yielding less than 320 mAh g^{-1} at 1 C and 200 mAh g^{-1} at 10 C [46–48]. Consequently, there is a pressing need for developing low-cost, environmentally friendly synthesis methods that result in MXenes with well-ordered terminal functional groups, which are essential for optimizing their performance in energy storage applications.

Recent advancements have sought to enhance the traditional preparation methods through milder etching techniques, such as “wet etching without fluoride” and “molten-salt etching.” Ammonium hydroxide has been utilized to facilitate the selective removal of aluminum without introducing fluoride [65]. While these methods show promise, they still tend to leave MXenes with surface terminations that may not provide the desired electronic properties and therefore require further refinement. The focus on tailoring terminal groups, particularly with sulfur and selenium terminations, has garnered attention due to their superior conductivity compared to oxygen-terminated MXenes [53, 66–68]. Research has demonstrated that carbon-free one-pot synthesis methods can effectively produce S/Se-terminated MXenes with enhanced charge transport properties, thus enabling faster electron and ion mobility essential for high-performance battery applications.

Electrode composite materials incorporating various metal and non-metal elements with diverse metal-anion bonding covalency exhibit substantial potential for fast-charging applications. This is achieved through modulation of electronic structures,

facilitation of multiple redox centers, enhancement of charge-transfer kinetics, and integration of intercalation alongside conversion/alloying-type storage processes.

To evaluate the appropriate band positioning in these materials, the on-site Coulomb interaction energy (U) is employed to address localized electron repulsion [69–71]. It is commonly accepted that U is inversely related to orbital volume, suggesting that U increases across transition metals within the same period (from Ti^{n+} to Ni^{n+}) due to orbital contraction, while it decreases from 3d to 5d elements as a result of orbital expansion. The charge-transfer term (Δ) is intricately linked to the electronegativity difference between the metal (M) and the anion (X), representing the energy difference between the bonding ($M - X$) and antibonding ($M - X$) molecular orbitals.

In situations where U is much smaller than Δ ($U \ll \Delta$) and falls within the Mott-Hubbard region, a significant Coulomb repulsion (U) leads to the bifurcation of transition-metal d states into lower and upper Hubbard bands (LHB and UHB), creating a Mott-Hubbard gap across the Fermi level. Metals with d0 configurations (e.g., Ti^{4+} , V^{5+} , Nb^{5+}) typically establish robust $M - X$ frameworks during the cationic redox processes that occur during battery discharge and charge (**Figure 1a**). The bonding of d0 metals with anions does not provide the filled antibonding orbitals necessary for anionic redox reactions during charging, thereby promoting structural stability [72–74].

When analyzing the case where U exceeds Δ ($U > \Delta$), the bandgap in the charge-transfer region correlates with variations in electronegativity differences between cation and anion, suggesting that the oxidation of M during charging elevates the U value, while the reduction during discharge generally lowers it. Introducing a second metal ($M2$) with a high U value into the $M1 - X$ framework can result in the overlap between the lower Hubbard band ($M2 - X$) and the non-bonding X p band, indicating the formation of covalent bonds in $M2 - X$ (**Figure 1b,c**). During discharge, as electrons are injected, the overlap between the ($M2 - X$) band and X p orbitals diminishes, inducing a weakening of the $M - X$ covalent bonds due to the reduced U value. The formation of a partially filled ($M2 - X$)* band can enhance redox pseudocapacitance, as cations continue to gain electrons during discharge, resulting in bond breakage and potential alloying.

In scenarios where U is significantly larger than Δ ($U \gg \Delta$), the presence of non-bonding X p states above the filled LHB generally prompts reductive decoupling of the anion from the framework, leading to the generation of $(X - X)^{n-}$ species and potentially the release of X_2 [75, 76]. The coupling of $X - X$ dimers with transition metals may prevent metal agglomeration, thus maintaining structural integrity during cycling. Therefore, the covalent interactions of $M2 - X$ bonds can facilitate the use of alloying-type metals such as Ge, Ga, In, and Sn in energy storage systems, enhancing their pseudocapacitance behavior.

In addition to the bimetal modulation strategy for optimizing metal-anion bonding covalency, incorporating (bi)anions with varying electronegativities allows for significant alterations in orbital hybridization of $M - X$ bonds. Generally, substituting anions with larger, more polarizable “soft” alternatives having lower electronegativity can enhance the integration of the anionic p band into the metallic d band, thereby promoting improved covalent mixing of the orbitals and enhancing electronic conductivities (**Figure 1d**) [77]. Such improvements in electronic conductivities have been noted in chalcogenides such as TiS_2 , $TiSe_2$, and $TiTe_2$, which exhibit distinct semiconductor, semimetal, and metallic characteristics, respectively [78, 79]. Conversely, substituting with a smaller “hard” element, like fluorine, which has high electronegativity, tends to diminish $M - X$ hybridization, thereby improving the redox potential and suppressing cation plating.

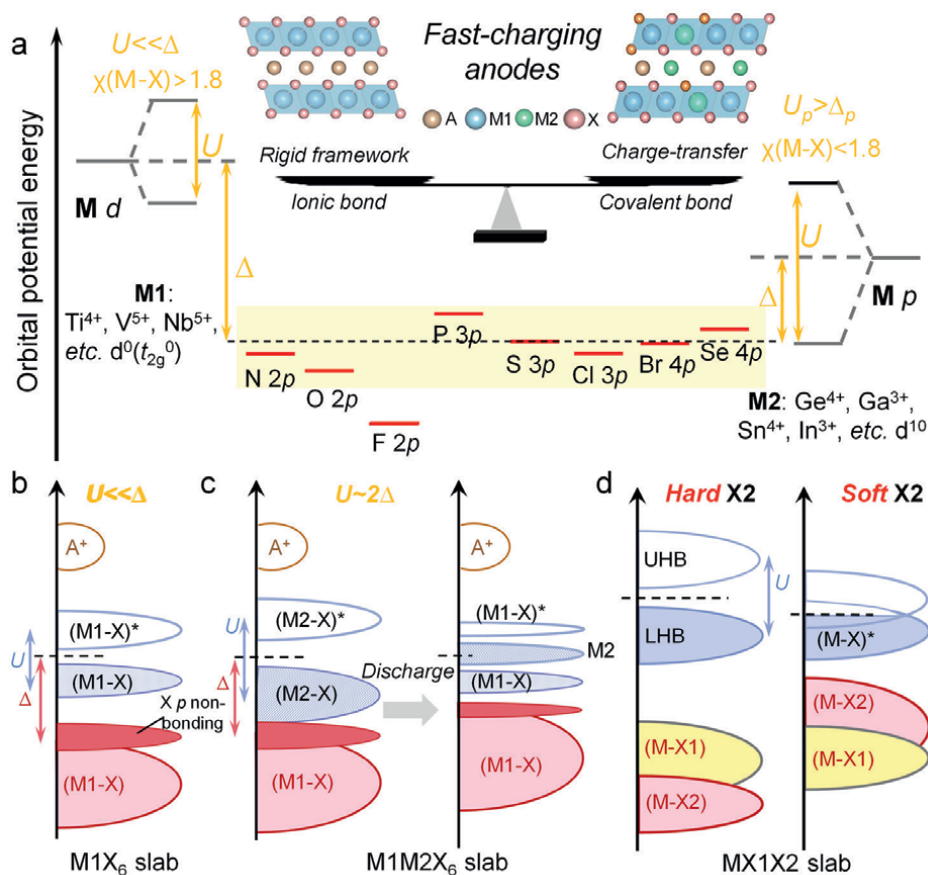


Figure 1. (a) Energy diagrams illustrating the charge-transfer ($U > \Delta$) and Mott-Hubbard ($U \ll \Delta$) mechanisms for the development of integrated M1M2X_n electrodes, featuring a robust framework and alloy-type metals. U denotes the on-site Coulomb interaction energy, Δ represents the charge-transfer term, X signifies non-metal elements, M indicates transition metal elements, and A denotes alkaline metal elements. The term $\chi(M-X)$ reflects the electronegativity difference between M and X . (b) Band structure analysis of the M1X₆ configuration, demonstrating effective electron injection without interference between (M1-X) and X p non-bonding states. (c) Band structure of the M1M2X₆ configuration under discharge conditions ($U > \Delta$), revealing the overlap between (M2-X) and X p non-bonding states, alongside the reduction of M2 metal. (d) Band structure of MX1X2 compositions, such as Ti₃C₂O₂ and Ti₃C₂S₂, highlighting Mott-Hubbard splitting effects. The terms hard and soft X2 refer to non-metal elements characterized by higher and lower electronegativity, respectively, compared to the original X1 non-metal element. Reproduced from ref. [44], copyright ACS.

3. MXene preparation and terminated groups characterization

Traditional synthesis approaches typically involve the selective etching of A elements (group IVA or IIIA, such as Al) from MAX phase materials using acidic or alkaline solutions. The top-down synthesis of MXenes frequently leads to disordered surface terminations, including hydroxyl (-OH), oxygen (-O), and fluoride (-F), which can adversely affect their electrochemical properties and result in suboptimal lithium-ion storage capacities, usually below 150 mAh·g⁻¹ [46–48], due to impaired electronic conductivity and diminished chemical stability [49, 50, 64].

Preliminary studies suggest that Cl/O-terminated Ti_3C_2 MXene, when synthesized without F- and OH-terminals, may exhibit superior lithium storage capacities. Theoretically, substituting terminal groups from –O to –Se enhances the overlap of the lower Hubbard band (LHB) and empty upper Hubbard band (UHB), facilitating electron mobility between occupied and unoccupied metallic bands. Building on

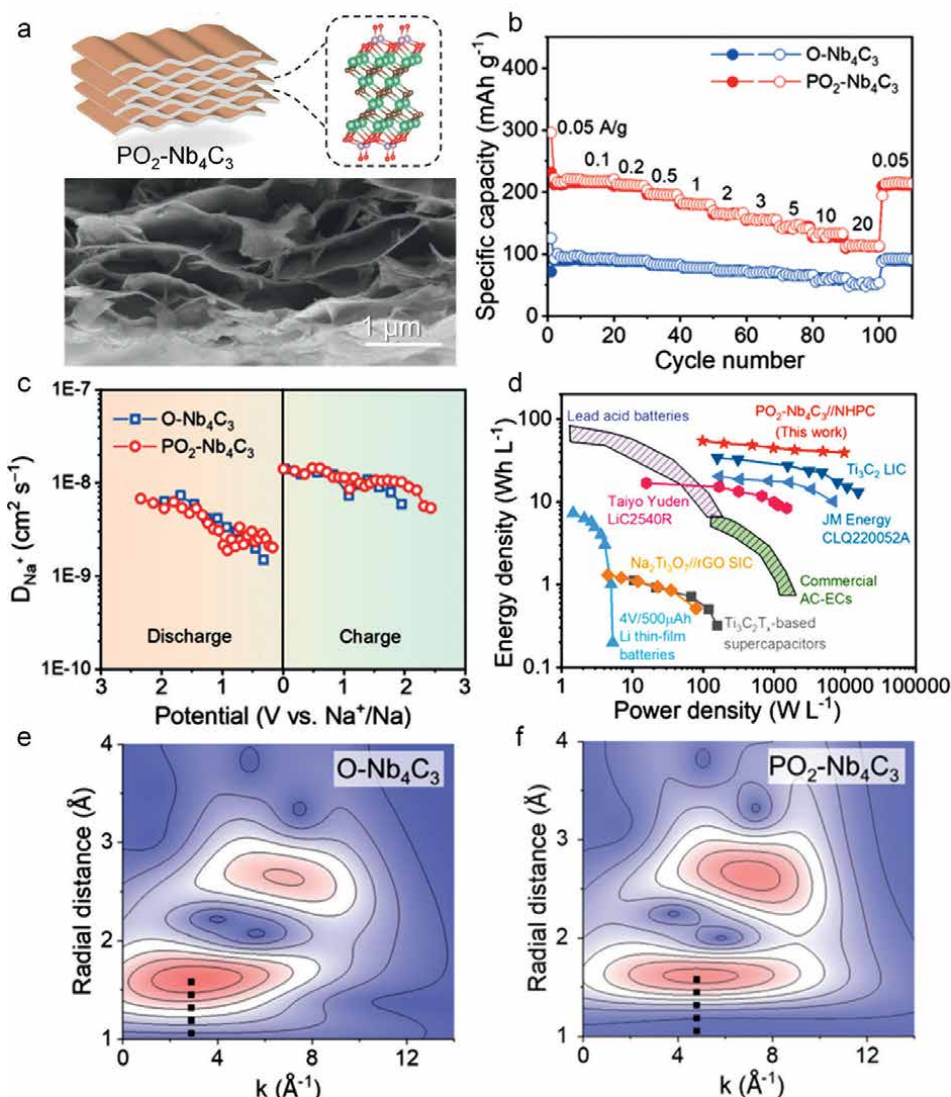


Figure 2. (a) Structural representation of MXenes, highlighting the arrangement of transition metal and non-metal elements. (b) Energy barrier profiles for Na^+ diffusion in $\text{Ti}_3\text{C}_2\text{O}_2$ and $\text{Ti}_3\text{C}_2\text{O}_{1.85}\text{N}_{0.17}$, emphasizing the impact of terminal groups on ionic conductivity. (c) Diagrammatic overview of solid electrolyte interphase (SEI) formation and the associated charge-transfer barriers on Ti_3C_2 and $\text{Ti}_3\text{C}_2\text{-N}$ electrodes, adapted from ref. [80], under a Creative Commons CC-BY License, Springer open. (d) Schematic representation and scanning electron microscopy (SEM) image of the $\text{PO}_2\text{-Nb}_4\text{C}_3$ structure, illustrating tailorable terminal functionalities. (e) Ragone plots comparing the performance of the $\text{PO}_2\text{-Nb}_4\text{C}_3$ sodium-ion capacitor with various energy-storage systems, including lithium capacitors (LiC). (f) Wavelet-transformed extended X-ray absorption fine structure (EXAFS) spectra for $\text{O-Nb}_4\text{C}_3$ and $\text{PO}_2\text{-Nb}_4\text{C}_3$, illustrating the structural dynamics, adapted from ref. [61], copyright Wiley-VCH.

this, Zhenbo Wang and colleagues developed a nitrogen-terminated Ti_3C_2 MXene ($\text{Ti}_3\text{C}_2 - \text{N}$) aimed at enhancing sodium-ion storage kinetics for fast-charging applications [80]. These studies have demonstrated a significant reduction in Na^+ diffusion energy barriers upon nitrogen substitution (**Figure 2b**), facilitating solvent and Na^+ co-intercalation at lower temperatures, which effectively lowers the desolvation energy barrier and fosters the formation of an inorganic-dominated solid electrolyte interphase (SEI) with reduced charge-transfer resistance (**Figure 2c**). The addition of well-ordered nitrogen terminals increases interlayer spacing, enhances electronic conductivity, and provides extra adsorption sites for Na^+ , collectively improving both capacity and rate performance. Furthermore, Xinliang Feng et al. introduced a redox-active phosphorus–oxygen terminal MXene ($\text{PO}_2 - \text{Nb}_4\text{C}_3$), which exhibits substantially increased specific capacities for swift sodium storage (**Figure 2d**) [61]. Compared to its O-terminated counterpart ($\text{O} - \text{Nb}_4\text{C}_3$), the $\text{PO}_2 - \text{Nb}_4\text{C}_3$ delivered a remarkable increase in cycle life with negligible capacity fading after 2000 cycles, achieving a doubled sodium storage capacity of 221 mAh g^{-1} and achieving fast-charging performance with retention of 80% capacity in just 4.9 minutes. Enhanced redox activity and additional Nb redox sites, as revealed by X-ray photoelectron spectroscopy (XPS), significantly contribute to this increased capacity.

Interestingly, the Na^+ diffusion coefficient of $\text{PO}_2 - \text{Nb}_4\text{C}_3$, assessed using galvanostatic intermittent titration technique (GITT), was found to be comparable to that of $\text{O} - \text{Nb}_4\text{C}_3$, indicating that replacing terminal groups with larger species does not impede Na^+ diffusion kinetics. When paired with hierarchically porous N-doped carbon cathodes, this $\text{PO}_2 - \text{Nb}_4\text{C}_3$ -based Na^+ capacitor could deliver impressive energy densities (55 Wh L^{-1}) alongside supercapacitor-level power densities ($\sim 9800 \text{ W L}^{-1}$), thereby meeting the stringent demands for high-rate and high-capacity energy storage devices (**Figure 2e**). Notably, the X-ray absorption fine structure (EXAFS) spectra demonstrated a shift in the Nb – C(O) peak from $3.0 \text{ \AA}^{-1}$ for $\text{O} - \text{Nb}_4\text{C}_3$ to $4.8 \text{ \AA}^{-1}$ for $\text{PO}_2 - \text{Nb}_4\text{C}_3$, indicating an increase in Nb – C(O) bond length following the PO_2 substitution (**Figure 2f**).

Inspired by the structures of transition metal dichalcogenides (TMDs), recent advancements have introduced innovative one-step Lewis-acid organic-assisted etching method that streamline the synthesis process while promoting the formation of ordered terminal groups (**Figure 3a**) [81, 82]. This structure can be conceptualized as substituting the M layer in TMDs with the [M–C–M] layer characteristic of MXenes. The use of selenium terminals takes full advantage of the excellent conductivity inherent in the [Nb–C–Nb] layer, while also providing enhanced electrochemical activity unattainable with conventional O-containing terminations. The one-step method for synthesizing Nb_2CSe_2 involved a straightforward procedure where niobium, carbon, and selenium powders, along with minimal hexachlorobenzene (C_6Cl_6), were heated. This process avoids the need for acidic or molten-salt treatment, simplifying the preparation and enhancing yield, which can reach up to 99 wt.%. Alternative approaches to enhance the efficiency of MXene synthesis involve utilizing lighter transition metals (e.g., Ti, V, Cr) or incorporating catalysts to facilitate metal gasification, effectively lowering synthesis temperatures and costs [82]. Additionally, strategies that involve creating low-temperature intermediates, which can be easily removed through mild etching processes such as copper pre-intercalation have shown promise in improving purity and compatibility for subsequent applications [82]. The introduction of orderly terminating selenium groups significantly elevates the material's conductivity—measured to be approximately 2000 times higher ($7.14 \times 10^4 \text{ S m}^{-1}$) than that of conventional Nb_2CT_x MXene, which has disordered surface terminations,

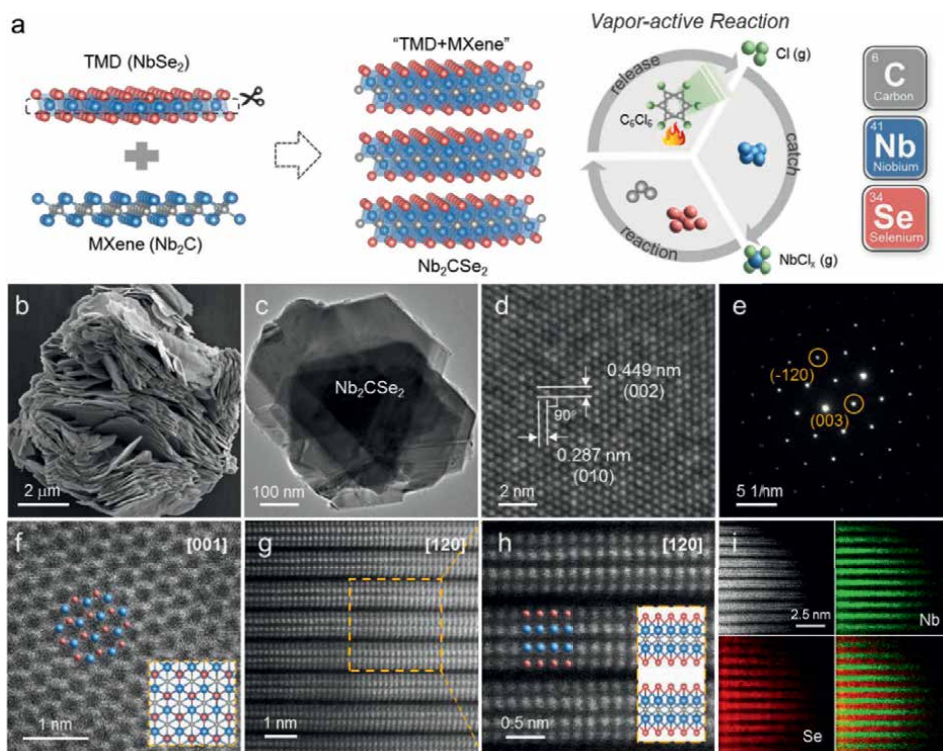


Figure 3.

(a) Schematic representation of the one-step synthesis of Nb_2CSe_2 via a “vapor-active reaction,” showcasing an efficient approach to developing MXenes with tailored terminal groups. (b) Scanning electron microscopy (SEM) image revealing the surface morphology of Nb_2CSe_2 . (c) Transmission electron microscopy (TEM) image providing insights into the structural features. (d) High-resolution transmission electron microscopy (HRTEM) image illustrating atomic-scale details, while (e) selected area electron diffraction (SAED) patterns confirm crystallinity. High-angle annular dark field (HAADF) atomic images of Nb_2CSe_2 captured along (f) the [001] crystal direction and (g, h) the [120] crystal direction, highlighting the arrangement of transition metals and non-metals. (i) Energy dispersive spectroscopy (EDS) elemental mapping images illustrating the distribution of [Se-Nb-C-Nb-Se] layers, emphasizing the influence of terminal groups on electronic properties vital for fast-charging applications. Reproduced from ref. [81], copyright Elsevier.

and it enhances carrier concentration approximately 1900 times ($1.85 \times 10^{21} \text{ cm}^{-3}$). Furthermore, these redox-active selenium terminals introduce additional active sites, boosting lithium-ion storage capacity to 390 mAh g^{-1} at 1 C and 270 mAh g^{-1} at 10 C. The high-rate capability of Nb_2CSe_2 is evident with a stable output of 170 mAh g^{-1} at 50 C, significantly surpassing the performance of most reported MXenes and TMD-based anode materials [83]. Notably, the Nb_2CSe_2 electrode can maintain a reversible capacity of 160 mAh g^{-1} over 6500 cycles at 25 C, showcasing exceptional structural stability [81]. During the vapor-active reaction, C_6Cl_6 decomposes at elevated temperatures, producing halogen-containing gases that react with niobium to form NbCl_x species. These gaseous NbCl_x molecules effectively interact with carbon and selenium atoms, resulting in the formation of the layered ternary compound Nb_2CSe_2 , while chlorine is released, facilitating a continuous “catch-reaction-release” cycle throughout the synthesis. The surface [Nb-Se] layers provide enhanced pseudocapacitance for energy storage, akin to TMD materials, while the Se terminations fully leverage the conductivity of the [Nb-C] layers. The prepared Nb_2CSe_2 nanoflakes exhibit a distinct layered morphology (Figure 3b), favoring hexagonal sheet formation (Figure 3c).

High-resolution transmission electron microscopy (HRTEM) imaging depicts lattice fringes corresponding to the (010) and (002) planes, with distances measuring 0.287 nm and 0.449 nm, respectively (**Figure 3d**). Selected area electron diffraction (SAED) patterns confirm the crystalline structure through observable (−120) and (003) planes (**Figure 3e**). High-angle annular dark field (HAADF) scanning transmission electron microscopy (STEM) images demonstrate a distinct hexagonal pattern, with atoms showing varying contrast—stronger contrasts attributed to Nb and weaker to Se, consistent with the hexagonal assembly of Nb₂CSe₂ (**Figure 3f**). Cross-sectional images reveal a layered structure with an approximate thickness of ~1 nm (**Figure 3g**). Each [Nb-C-Nb] layer is systematically terminated with selenium atoms, forming the [Se-Nb-C-Nb-Se] arrangement (**Figure 3h**). Van der Waals forces connect these sandwich-like layers, resulting in an interlayer distance of approximately 0.318 nm. Energy dispersive spectroscopy (EDS) analysis further confirms the elemental distribution, illustrating a patterned arrangement of Nb (green) and Se (red) layers (**Figure 3i**). Integrating ordered, soft anionic terminal groups into MXene structures enhances electronic conductivity and mitigates internal stress during cation insertion and extraction, thereby enabling reliable and rapid charging. The one-step preparation method for Se-terminated Nb₂CSe₂ represents a significant advancement in designing MXenes for fast-charging applications, markedly improving electronic conductivity and electrochemical performance through strategic terminal group engineering, which addresses the energy-power trade-off in conventional energy storage devices.

4. Electrochemical and thermal properties of specific groups terminated MXenes

MXenes are emerging as highly promising materials in energy storage and management due to their exceptional electrical conductivity, mechanical properties, and adaptability through terminal group functionalization. Specific ordered terminations have been found to significantly influence the thermal and electronic properties of MXenes, paving the way for enhanced performance in advanced applications [30–34]. Among the diverse MXene compositions, the functionalization with specific terminal groups, such as selenium and sulfur, has been shown to significantly enhance their electrochemical properties. The electrochemical properties of Se-terminated Nb₂CSe₂ and conventional Nb₂CT_x MXene were comprehensively evaluated within a voltage range of 0.01–3 V. **Figure 4a** presents the galvanostatic charge–discharge (GCD) profiles of Nb₂CSe₂ at a rate of 0.5 C (1 C = 200 mA g^{−1}) over the initial three cycles [81]. The Nb₂CSe₂ electrode achieved an initial discharge capacity of 941 mAh g^{−1} and a charge capacity of 503 mAh g^{−1}, resulting in an initial Coulombic efficiency (ICE) of 53.4%. The slight decline in capacity observed during the initial cycles is attributed to the formation of a stable SEI layer, a common phenomenon in battery materials [82, 84]. In contrast, the Nb₂CT_x electrode exhibited a significantly lower charge capacity of 383 mAh g^{−1} during its first cycle, underscoring the superior performance of Nb₂CSe₂. Further testing of the rate capabilities of Nb₂CSe₂ and Nb₂CT_x electrodes indicated remarkable high-rate performance and structural robustness of Se termination (**Figure 4b**). Long-term stability at elevated rates was also examined. Cyclic performance assessments revealed that the Nb₂CSe₂ electrode exhibited a stable discharge capacity of 265 and 160 mAh g^{−1} after 2400 and 6500 cycles at high rates of 10 and 25 C, respectively (**Figure 4c**). By analyzing the relationship between peak currents (I) and sweep rates (v) through the equations:

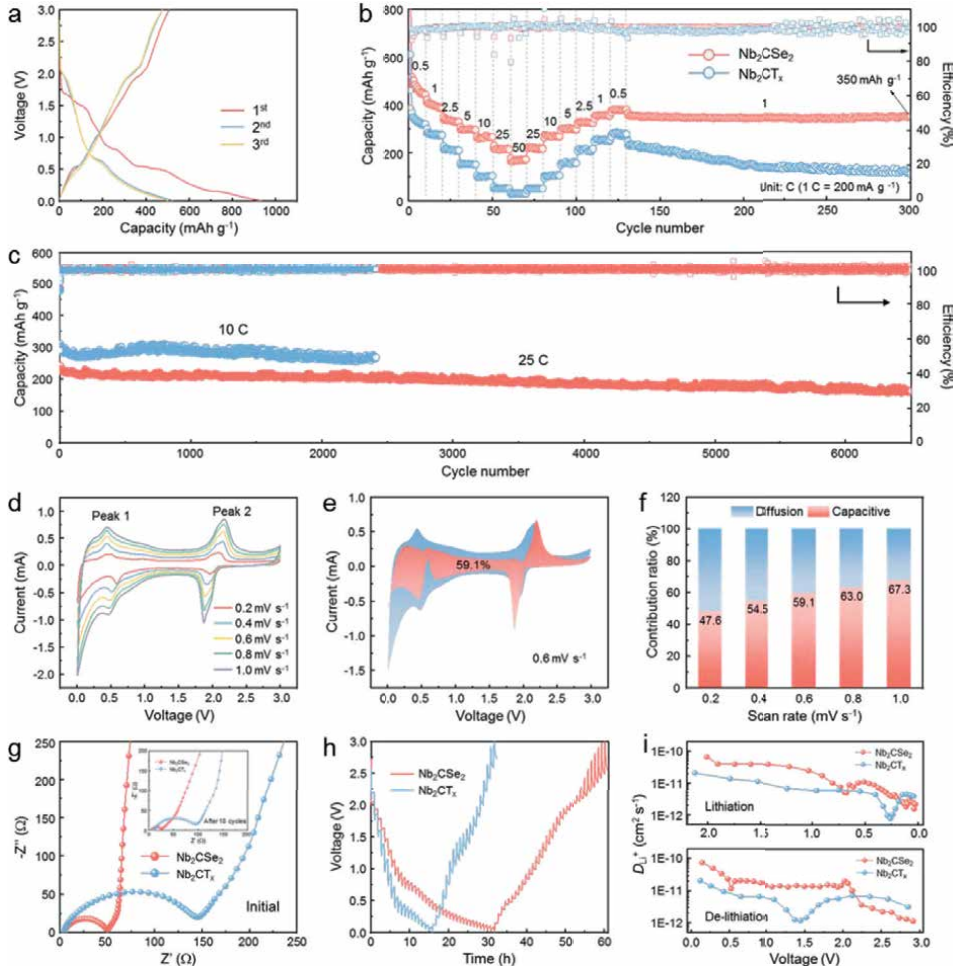


Figure 4. (a) Galvanostatic charge-discharge (GCD) curves of Nb₂CSe₂ over the first three cycles, illustrating initial performance characteristics. (b) Comparative rate performance of Nb₂CSe₂ and Nb₂CT_x, highlighting the impact of terminal groups on ionic conductivity and overall energy storage efficiency. (c) Long-term cycling stability of Nb₂CSe₂ assessed at current densities of 10 and 25 C, demonstrating its reliability for fast-charging applications. (d) Cyclic voltammetry (CV) curves of Nb₂CSe₂ obtained at various scan rates, reflecting electrochemical behavior. (e) Capacitive contributions of Nb₂CSe₂ at a scan rate of 0.6 mV s⁻¹, emphasizing the role of pseudocapacitance in energy storage. (f) Evaluation of pseudocapacitive contributions across different scan rates, providing insight into the reaction kinetics. (g) Nyquist plots of Nb₂CSe₂ and Nb₂CT_x at the initial stage and after 10 cycles, illustrating changes in charge transfer resistance and ionic transport properties. (h) Galvanostatic intermittent titration technique (GITT) potential profiles of Nb₂CSe₂ and Nb₂CT_x, shedding light on their dynamic behavior during lithium-ion diffusion. (i) Li⁺ diffusion coefficients of Nb₂CSe₂ and Nb₂CT_x derived from GITT measurements, reinforcing the influence of tailored terminal groups on fast lithium transport. Reproduced from ref. [81], copyright Elsevier.

$$i(V) = av^b \quad (1)$$

The b values were calculated for Peak 1 and Peak 2 to be 0.80 and 0.88, respectively, revealing a predominance of fast capacitive-controlled kinetics, correlating with the enhanced fast-charging capabilities of Nb₂CSe₂ (Figure 4d) [54, 55]. At a scan rate of 0.6 mV s⁻¹, the capacitive contributions accounted for 59.1% of the

total capacity (**Figure 4e**). As scan rates increased, the capacitive component grew from 47.6% to 67.3%, demonstrating a shift towards enhanced capacitive behavior (**Figure 4f**). The charge transfer resistance (R_{ct}) for pristine Nb_2CSe_2 was measured at 50.1 Ω , significantly lower than the 148.4 Ω exhibited by Nb_2CT_x (**Figure 4g**). The Nb_2CSe_2 electrode's steep slope in the low-frequency region indicates its capacitive-like behavior. After 10 cycles, the R_{ct} for Nb_2CSe_2 decreased further to 26 Ω , while R_{ct} for Nb_2CT_x increased to 100 Ω (inset of **Figure 4g**). Galvanostatic intermittent titration technique (GITT) measurements confirmed that the overpotential values for Nb_2CSe_2 were consistently smaller than those for Nb_2CT_x (**Figure 4h**), with calculated diffusion coefficients indicating superior lithium-ion diffusion kinetics for Nb_2CSe_2 (**Figure 4i**). These kinetic analyses highlight the rapid charge-transfer process facilitated by the selenium terminal groups, significantly enhancing ion and electron transport.

Traditional synthesis of MXenes with specialized terminal groups involves a multi-step process that includes the preparation of a MAX phase precursor, followed by high-temperature solid-state reactions and chemical etching using acids or molten salts. This conventional methodology often leads to issues such as metal impurities from incomplete etching, the generation of hazardous acidic waste containing fluorides, and generally low product yields (**Figure 5a**) [62–68]. To address these challenges, by introducing hexachlorobenzene (C_6Cl_6) into the synthesis process, there exists a unique ability to produce gas-phase metal chlorides such as $NbCl_x$ that participate in homogeneous reactions with gaseous nitrogen or oxygen at elevated temperatures, resulting in the formation of MXenes during the annealing phase (**Figure 5b**). This approach not only simplifies the preparation and reduces costs but also minimizes impurities, allowing for the inexpensive synthesis of S/Se-terminated MXenes with high yields and robust structural integrity suitable for large-scale production (**Figure 5c**).

Density of states (DOS) profiles reveal that Nb_2CSe_2 exhibits a dominant Nb d band at the Fermi level, surpassing that of Nb_2O_2C . This characteristic indicates enhanced electron transport properties for Se-terminated MXenes. The presence of Se terminals lowers the energy of the Nb d band and enhances the overlap between the filled lower Hubbard bands and the unoccupied upper Hubbard bands. This electronic structure facilitates greater redox activity of Nb in Nb_2CSe_2 , which is crucial for improved energy storage performance associated with the Se terminals. Investigating the thermal management capabilities of tailored terminal groups, measurements of temperature-dependent resistivity using a physical properties measurement system (PPMS) indicated that the electrical resistivity of Nb_2CSe_2 is 0.014 $\Omega \cdot mm$ at 298 K, significantly lower than that of Nb_2CT_x (30.60 $\Omega \cdot mm$) (**Figure 5d**). The resistivity of Nb_2CSe_2 exhibits a decrease with lowering temperature, confirming its metallic nature, while Nb_2CT_x displays semiconductor characteristics with a bandgap of approximately 1.47 eV [69, 70]. Remarkably, the electrical conductivity of Nb_2CSe_2 reaches $7.1 \times 10^4 S \cdot m^{-1}$, which is approximately 2184 times greater than that of Nb_2CT_x ($3.3 \times 10 S \cdot m^{-1}$) under ambient conditions. Further characterization via Hall effect measurements confirmed linear relationships between the Hall resistance (R_{hall}) values of Nb_2CSe_2 and Nb_2CT_x (**Figure 5e**). The slope for Nb_2CSe_2 ($-9.39 \times 10^{-3} m\Omega \cdot T^{-1}$) was found to be five orders of magnitude smaller than that of Nb_2CT_x ($-1.60 \times 10^{-2} \Omega \cdot T^{-1}$), indicating a far greater carrier concentration of approximately $1.9 \times 10^{21} cm^{-3}$ compared to $9.78 \times 10^{17} cm^{-3}$ for Nb_2CT_x . The importance of thermal management for battery applications is underscored by observations of thermal emission characteristics. According to Wien's displacement law, the peak wavelength (λ) of thermal radiation from a black body is

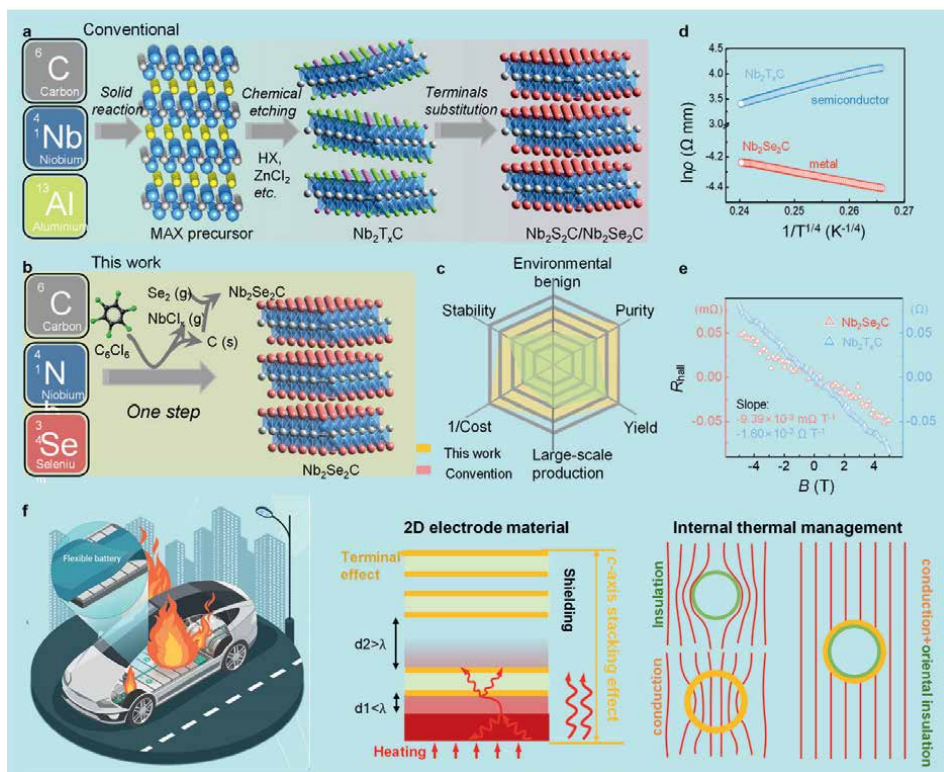


Figure 5.

Characterizations of S/Se-terminal MXenes synthesized using a cost-effective one-step method. (a) Schematic representation of traditional synthesis routes for S/Se-terminal MXenes, illustrating the limitations of multi-step processes. (b) Overview of the innovative one-step approach for synthesizing S/Se-terminal MXenes, emphasizing its efficiency and scalability. (c) Radar plots summarizing the key advantages of the one-step method, including cost-effectiveness, time efficiency, and improved material properties. (d) Measurement of electrical resistivity in S/Se-terminal MXenes, highlighting their conductive properties essential for fast-charging applications. (e) Field-dependent magnetization data at 298 K, examining the magnetic behaviors that may influence electrochemical performance. (f) Description of an internal thermal management strategy for flexible batteries, focusing on electrode design, which accounts for terminal and stacking effects. The interplane distance (d_1) and interflake distance (d_2) are critical; when the interflake distance exceeds the peak thermal wavelength (λ), it provides a thermal radiation shield, while an interplane distance below λ enhances near-field radiative heat transfer. Notably, within the temperature range of 300–500 K, the peak thermal emission wavelength falls between 5.8–9.6 μm , primarily in the mid-infrared range (3–8 μm). Reproduced from ref. [82], copyright Wiley-VCH.

inversely related to its absolute temperature (T), where $\lambda = b/T$ and b is the constant equal to $2.897 \times 10^{-3} \text{ m}\cdot\text{K}$. Operating within a temperature range of 300–500 K, the peak thermal emission wavelengths span from 5.8 to 9.6 μm , predominantly within the mid-infrared spectrum (3–8 μm). Consequently, the development of materials exhibiting high reflectivity in the mid-infrared range is critical for mitigating thermal transfer challenges. Leveraging the properties of 2D MXene materials for internal thermal management in flexible batteries necessitates strategic optimization of terminal groups and interlayer spacing to shield against thermal radiation while enhancing near-field radiative heat transfer capabilities (**Figure 5f**) [71]. The substantial interlayer distances in MXenes typically exceed the peaks in thermal wavelength, enabling effective thermal radiation shielding.

To investigate the impact of terminal groups on infrared (IR) spectral selectivity, density functional theory (DFT) calculations were conducted on Nb_2CSe_2 and

$\text{Nb}_2\text{O}_2\text{C}$ to evaluate their optical properties in the mid-infrared and near-infrared regions. **Figure 6a** illustrates the dielectric function, where ϵ_1 represents the real part associated with polarization, and ϵ_2 denotes the imaginary part related to energy dissipation dynamics within the materials [77, 78]. Notably, Nb_2CSe_2 exhibited a significantly enhanced dielectric function in the mid-IR range compared to $\text{Nb}_2\text{O}_2\text{C}$, indicating a marked difference in their intrinsic polarization and absorption characteristics linked to the nature of their terminal groups. The interaction of the nanoflakes' orientations, particularly along the z-direction, with near-IR absorption and electrical conduction was also examined (**Figure 6b,c**). This finding underscores the critical interplay between stacking effects and their ability to absorb and conduct near-IR radiation [24]. By substituting the disordered terminal groups (O/OH/F) in Nb_2CT_x with Se terminals, the electronic conductivity was markedly improved. Additionally, this substitution significantly influenced the carrier mobility and migration within the material, which has implications for thermal conductivity.

Moreover, the energy loss function—a valuable metric for assessing electron dynamics—was analyzed to quantify the energy losses incurred when electrons rapidly penetrate the electrodes. As depicted in **Figure 6d**, $\text{Nb}_2\text{O}_2\text{C}$ presented a prominent energy loss of approximately 2.2 eV along the z-direction, whereas Nb_2CSe_2 exhibited minimal energy loss. This difference is likely indicative of Nb_2CSe_2 's metallic character, which facilitates more efficient electron transport. In thermal management, the mid-infrared reflectivity of Nb_2CSe_2 surpassed that of $\text{Nb}_2\text{O}_2\text{C}$ in the lower

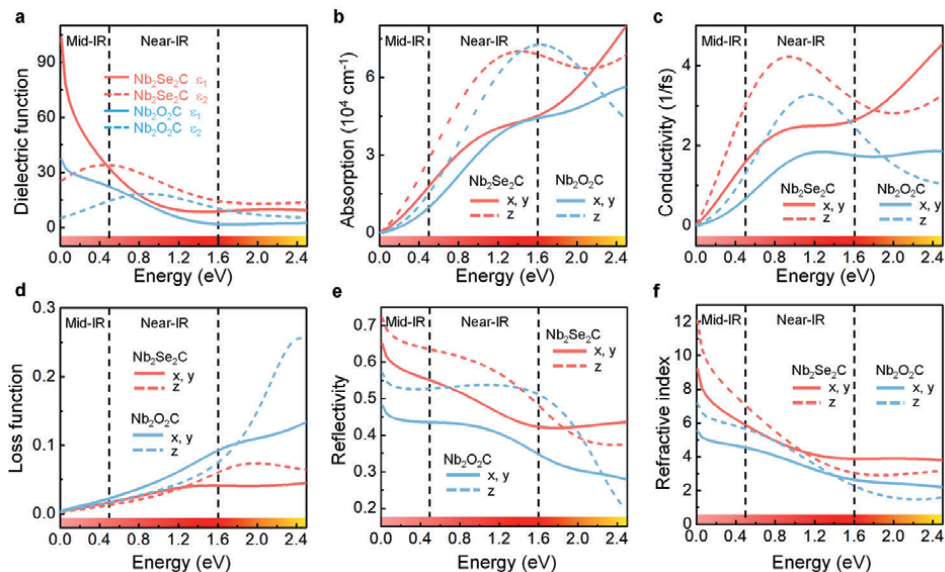


Figure 6. Influence of terminal groups and flake orientation on the optical and electrical properties of MXenes. (a) Calculated dielectric function of Nb_2CSe_2 and $\text{Nb}_2\text{O}_2\text{C}$, reflecting the interaction of electromagnetic waves with these materials. (b) Absorption coefficients demonstrating how terminal modifications impact light absorption capabilities. (c) Conductivity measurements indicating the influence of terminal groups on charge transport efficiency. (d) Loss function profiles illustrating energy dissipation characteristics critical for fast-charging applications. (e) Reflectivity coefficients showing the extent of light reflectance, which can affect thermal management in energy storage systems. (f) Refractive index data revealing how terminal groups and crystal orientation alter optical performance. The analysis distinguishes between in-plane (xy) and out-of-plane ([00 l]) directions, emphasizing the role of structural orientation in tailoring the performance of MXenes for enhanced energy storage applications. Reproduced from ref. [82], copyright Wiley-VCH.

energy spectrum (**Figure 6e**). Significantly, Nb₂CSe₂ displayed greater spectral reflectivity along the z-direction compared to in-plane reflectivity, highlighting the importance of flake orientation in modulating thermal responses. Calculating the refractive index revealed that the integration of Se terminals, combined with specific flake orientations, leads to an augmentation of the refractive index (**Figure 6f**).

The DFT calculations corroborate the superior spectral selectivity of Nb₂CSe₂, validating the effects of terminal groups and flake orientation on the material's performance. The preferential alignment of Nb₂CSe₂ films parallel to filter paper during vacuum filtration contributes to optimal spectral selectivity. This effect is primarily attributed to the high permittivity offered by Se terminals and the directional enhancement of conductivity along the z-direction. The X-ray diffraction (XRD) pattern of Nb₂CSe₂ synthesized from graphite or carbon nanotubes (CNTs) reveals a distinct trigonal layered structure, with a spacing of 0.89 nm between the layers (**Figure 7a**). The synthesized Nb₂CSe₂ powders, when dispersed in anhydrous alcohol, exhibited a notable Tyndall effect, as illustrated in the inset of **Figure 7a**. Transmission electron microscopy (TEM) analysis confirmed the flaky morphology of Nb₂CSe₂ (**Figure 7b**), with the accompanying optical photograph exhibiting the high product yield achieved through the one-step synthesis method. The single-crystalline nature of Nb₂CSe₂ was further validated using high-resolution transmission electron microscopy (HRTEM) and corresponding selected area electron diffraction (SAED) patterns (**Figure 7c**). Elemental mapping images corroborated the presence of niobium (Nb), carbon (C), and selenium (Se) within the obtained samples. The preparation of Nb₂CSe₂/CNT or Nb₂CT_x/CNT films involved mixing Nb₂CSe₂ or Nb₂CT_x with CNTs followed by suction filtration, resulting in free-standing electrodes suitable for energy storage applications (**Figure 7d**). The Nb₂CSe₂/CNT films displayed flexibility, allowing them to be bent and folded without damage (**Figure 7e**), and exhibited an optimal thickness of approximately 6.7 μm (**Figure 7f**), positioning them as promising candidates for flexible energy storage devices [72–74].

To evaluate their thermal management capabilities, the prepared Nb₂CSe₂/CNT, Nb₂CT_x/CNT, and graphene oxide (GO) films were placed on a hot plate set at constant temperatures of 60, 100, and 150°C. The infrared (IR) images captured during this process revealed that the Nb₂CSe₂/CNT film appeared cooler than both Nb₂CT_x/CNT and GO films, indicating its significantly lower IR emissivity and thermal radiation (**Figure 7g**). Furthermore, upon applying an electrolyte to the surfaces of these films, thermal imaging indicated that the Nb₂CSe₂/CNT film maintained reduced thermal radiation even under elevated temperatures.

The enhanced thermal performance of Nb₂CSe₂ is attributed to the advantageous properties of Se terminal groups, which possess higher permittivity (ε) and superior electronic conductivity at room temperature (δ_{RT}). These factors collectively contribute to the low IR emissivity observed in Nb₂CSe₂ compared to O- or F-terminated MXenes (**Figure 7h**). Additionally, Nb₂CSe₂ exhibited characteristic diamagnetic behavior with negative susceptibility that remained consistent across temperature variations, whereas Nb₂CT_x showed paramagnetic behavior at 300 K due to a randomly oriented magnetic moment (**Figure 7i**). The paramagnetic susceptibility of Nb₂CT_x decreased with increasing temperature, following Curie's law, which is a result of thermal agitation [75, 76]. This thermal agitation in Nb₂CT_x contributes to higher thermal radiation and IR emissivity compared to Nb₂CSe₂. To further illustrate the thermal stability of these materials, electrolyte droplets were introduced onto different electrodes, all placed on a hot plate set to 220°C under an argon atmosphere. Notably, while smoke was observed when the electrolyte fell onto the surface of the

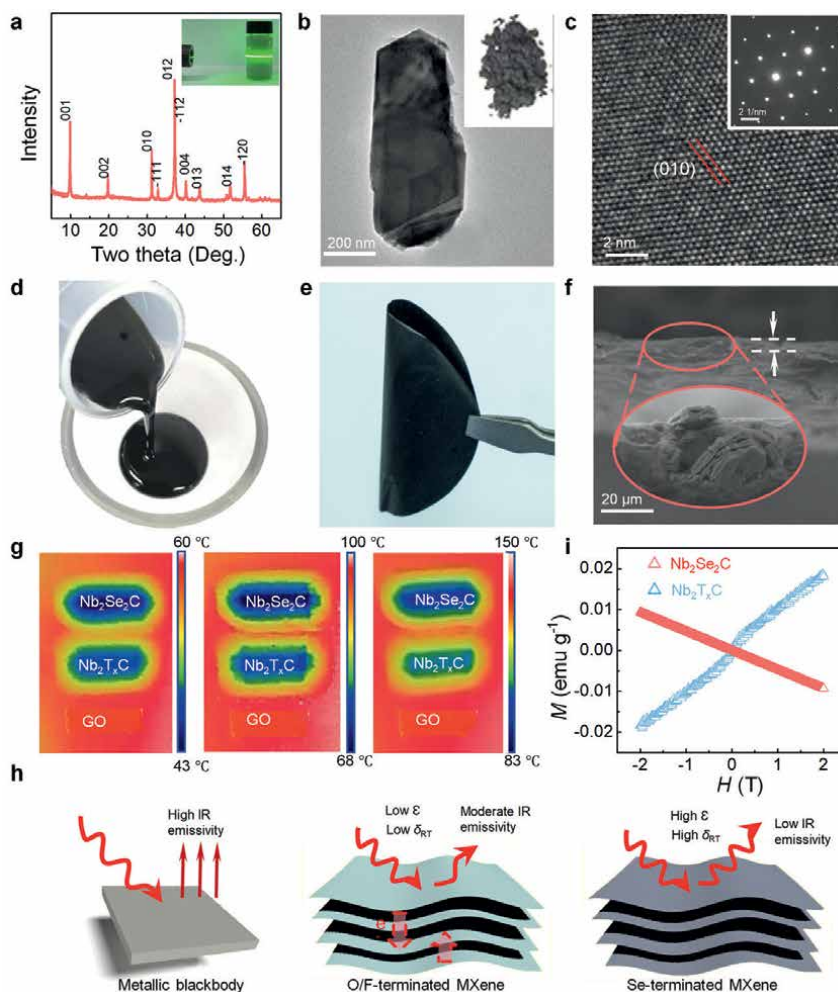


Figure 7. Infrared emissivity characteristics of $\text{Nb}_2\text{CSe}_2/\text{CNT}$ composite films. (a) X-ray diffraction (XRD) pattern showcasing the crystalline structure of Nb_2CSe_2 , with insets displaying optical images of the alcohol dispersion and the resulting Nb_2CSe_2 powders. (b) Transmission electron microscopy (TEM) image providing insights into the morphology of Nb_2CSe_2 , complemented by (c) high-resolution transmission electron microscopy (HRTEM) images revealing fine structural details. (d, e) Optical images of the flexible $\text{Nb}_2\text{CSe}_2/\text{CNT}$ film obtained via suction filtration, demonstrating the potential for flexible energy storage applications. (f) Cross-sectional scanning electron microscopy (SEM) image illustrating the layered architecture of the $\text{Nb}_2\text{CSe}_2/\text{CNT}$ film, which is critical for optimizing electrochemical performance. (g) Infrared photography comparing the thermal response of $\text{Nb}_2\text{CSe}_2/\text{CNT}$, $\text{Nb}_2\text{CT}_x/\text{CNT}$, and graphene oxide (GO) films on a hot plate set at temperatures of 60, 100, and 150 °C, highlighting the influence of terminal groups on thermal management. (h) Schematic illustrations depicting the structure of $\text{Nb}_2\text{CSe}_2/\text{CNT}$ films designed to possess low infrared emissivity, aiding in thermal regulation during operation. (i) Magnetic behavior analyses of Nb_2CSe_2 and Nb_2CT_x at 300 K, indicating the relationship between terminal function and magnetic properties relevant for the performance of energy storage devices. Reproduced from ref. [82], copyright Wiley-VCH.

pressed Super P electrode, the Nb_2CSe_2 electrode sustained the electrolyte droplets without significant reaction or smoke, demonstrating its superior thermal stability and safety characteristics.

The free-standing $\text{Nb}_2\text{CSe}_2/\text{CNT}$ film obtained through vacuum filtration was directly assembled into a flexible and bendable half-cell without needing a binder,

additive, or current collector (**Figure 8a**). The galvanostatic charge-discharge curves of the $\text{Nb}_2\text{CSe}_2/\text{CNT}$ electrodes at a current of 100 mA g^{-1} demonstrated a discharged specific capacity of 809.3 mAh g^{-1} (**Figure 8b**). The charge-discharge curves significantly overlapped, indicating the high cycling stability and reversibility of the electrode (**Figure 8c**). GITT measurements indicated improved Li^+ diffusion kinetics in the $\text{Nb}_2\text{CSe}_2/\text{CNT}$ composite (**Figure 8d**). Further charge transfer kinetics were analyzed using electrochemical impedance spectroscopy (EIS) (**Figure 8e**). The Nyquist plots for the electrodes consisted of a high-frequency semicircle and a low-frequency line, with the equivalent circuit represented as $R_s(\text{Qd}(\text{R}_{\text{ct}}\text{Qw}))$, where Qd is the double-layer capacitor, Qw is the Warburg diffusion element, R_s is the ohmic resistance, and R_{ct} denotes charge transfer resistance [79, 80]. Compared

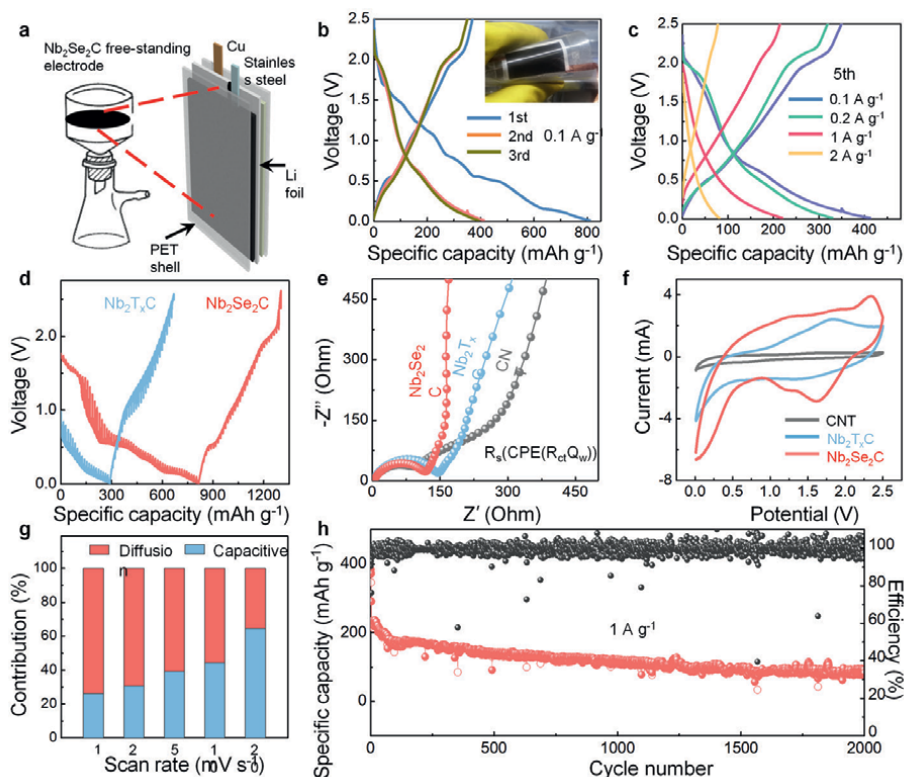


Figure 8.

Electrochemical performance assessment of flexible battery devices utilizing $\text{Nb}_2\text{CSe}_2/\text{CNT}$ composites. (a) Schematic illustration depicting the assembly process of the flexible batteries, highlighting the innovative use of a suction filtration technique, adapted from pngimg.com. (b) Galvanostatic charge-discharge curves for $\text{Nb}_2\text{CSe}_2/\text{CNT}$ flexible batteries at a current density of 100 mA g^{-1} , showcasing the initial electrochemical behavior. (c) Performance evaluation through galvanostatic charge-discharge curves at various current densities, demonstrating the adaptability of $\text{Nb}_2\text{CSe}_2/\text{CNT}$ batteries under different operational conditions. (d) Galvanostatic Intermittent Titration Technique (GITT) curves illustrating lithium-ion diffusion dynamics within the flexible battery structure. (e) Nyquist plots analyzing the electrochemical impedance of $\text{Nb}_2\text{CSe}_2/\text{CNT}$ and $\text{Nb}_2\text{CT}_x/\text{CNT}$ batteries, providing insights into charge transfer resistance which is crucial for fast-charging capabilities. (f) Cyclic voltammetry (CV) curves that characterize the electrochemical properties of the flexible batteries, indicating redox behavior and capacitive effects. (g) Evaluation of capacitive contributions of $\text{Nb}_2\text{CSe}_2/\text{CNT}$ flexible batteries recorded at varying scan rates, emphasizing the role of tailored terminal groups in enhancing charge storage mechanisms. (h) Cycling stability data showcasing the performance longevity of $\text{Nb}_2\text{CSe}_2/\text{CNT}$ flexible batteries, reflecting their reliability and suitability for fast-charging applications. Reproduced from ref. [82], copyright Wiley-VCH.

to Nb₂T_xC/CNT and CNT electrodes, the smallest semicircle diameter observed for Nb₂CSe₂/CNT indicated the fastest charge transfer kinetics. **Figure 8f** illustrates the cyclic voltametric curves of Nb₂CSe₂/CNT against Nb₂T_xC/CNT and CNT across 0.0–2.5 V. Nb₂CSe₂/CNT exhibited more pronounced cathodic peaks at approximately 1.75 V and 0.25 V, suggesting enhanced lithiation capacities. As the scanning rates increased, the contribution of surface capacitive-controlled processes rose from 26.3% at 1.0 mV s⁻¹ to 64.5% at 20.0 mV s⁻¹, indicating a shift from diffusion-dominated to surface capacitive-controlled processes at higher scan rates (**Figure 8g**) [61, 81]. Remarkably, the specific capacity remained around 80 mAh·g⁻¹ at a current density of 1.0 A g⁻¹ over 2000 cycles for the Nb₂CSe₂/CNT (**Figure 8h**). The design and implementation of tailored terminal groups in MXenes not only enhance their electrochemical performance but also significantly contribute to their functionality in thermal management for battery applications. This approach has the potential to optimize energy storage devices both in terms of efficiency and safety.

5. Conclusions

In this chapter, we have examined the promising role of surface-terminated MXenes as a transformative solution for enhancing the thermal management and electrochemical performance of metal-ion batteries. This innovative electrode exhibits its low mid-infrared emissivity and remarkable electrical conductivity, making it effective in minimizing heat generation and transfer within the electrode and organic electrolyte interfaces. Such properties are crucial for ensuring safe, high-rate energy storage.

Recent development of a one-step organic Lewis acid-assisted solid-state synthesis method for creating ordered S/Se-terminated MXenes presents a significant advancement over traditional fabrication techniques, such as HF etching and inorganic molten salts-assisted methods, which often introduce undesirable metal impurities and require complex multistage functionalization. This sustainable approach not only streamlines the production process but also maintains the integrity and performance of the resulting materials, paving the way for large-scale applications. The Se-terminated Nb₂CSe₂ electrode demonstrates exceptional electrochemical performance, achieving a specific capacity of 415 mAh·g⁻¹ at a current density of 100 mA·g⁻¹ by the fifth cycle and sustaining approximately 80 mAh·g⁻¹ over 2000 cycles at 1 A·g⁻¹. These remarkable enhancements arise from the introduction of additional redox sites from the selenium terminals, enhanced pseudocapacitive behavior, improved electronic conductivity, and excellent structural stability. Additionally, first-principles calculations indicate that the presence of Se terminals not only increases electronic density around the Fermi level but also enhances permittivity and conductivity in the mid-IR and near-IR regions, further contributing to efficient thermal management.

In summary, the strategic tailoring of terminal groups in MXenes offers a viable pathway to developing advanced electrodes that provide enhanced electronic conductivity, reduced thermal emissivity, and improved safety profiles. By leveraging these properties, next-generation metal-ion batteries can achieve high energy and power capabilities, effectively transforming the landscape of energy storage technologies. The insights and methodologies presented in this chapter not only underscore the importance of surface modification in MXene research but also set the stage for future exploration of 2D materials in the quest for efficient and safe energy storage solutions.

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Conflict of interest

The authors declare no competing interests.

Key terms

Mott-Hubbard Gap: Energy gap arising from electron-electron interactions in correlated materials.

Pseudocapacitance: Fast, surface-controlled charge storage mechanism.

Redox Activity: Electron transfer processes during charge/discharge.

Mid-IR Emissivity: Efficiency of thermal radiation emission in the 3–8 μm range.

A. Detailed synthesis procedure for Se-terminated Nb_2CSe_2 MXene

The one-step organic Lewis acid-assisted synthesis of Nb_2CSe_2 involves the following steps: Material Preparation: Niobium (Nb), carbon (C), and selenium (Se) powders are mixed in a molar ratio of 2:1:2. Hexachlorobenzene (C_6Cl_6) is added as a halogen source. Gas-Phase Reaction: The mixture is heated to 800–1000°C under argon flow. C_6Cl_6 decomposes into Cl_2 gas, which reacts with Nb to form volatile NbCl_x species. MXene Formation: NbCl_x reacts with C and Se vapors, forming layered Nb_2CSe_2 . Excess Cl_2 is evacuated, ensuring minimal impurities. Film Fabrication: The MXene powder is dispersed in ethanol and vacuum-filtered to create flexible, free-standing films.

B. Computational methods for DFT analysis

Density Functional Theory (DFT) calculations were performed using the Vienna Ab initio Simulation Package (VASP) with the following parameters: Exchange-Correlation Functional: Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA). Cutoff Energy: 500 eV. k-Point Grid: $6 \times 6 \times 1$ for monolayer structures. Convergence Criteria: Energy tolerance of 10^{-5} eV and force tolerance of 0.01 eV/Å. Van der Waals Correction: DFT-D3 method applied for interlayer interactions.

Acronyms

MXene	transition metal carbides/nitrides ($\text{M}_{n+1}\text{X}_n\text{T}_x$)
MIBs	metal-ion batteries

LIB	lithium-ion battery
NIB	sodium-ion battery
SEI	solid electrolyte interphase
GITT	galvanostatic intermittent titration technique
DFT	density functional theory
HRTEM	high-resolution transmission electron microscopy
XRD	X-ray diffraction

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An emerging family of two-dimensional transition-metal carbides and nitrides, known as MXenes, has become a focal point of materials research because of their exceptional electrical conductivity, tunable surface chemistry, mechanical properties, and solution-processability. This book offers a concise yet comprehensive overview of recent advances in MXene-based materials, emphasizing their design strategies, structure-property relationships, and technological relevance. The book covers key topics including flexible and wearable electronics, fiber-reinforced nanocomposites, neuromorphic and memory devices, biomedical applications, thin-film conductivity, and energy-storage systems with intrinsic thermal management. It highlights how surface engineering and interfacial interactions enable precise control over multifunctional performance across diverse material systems. By integrating perspectives from materials science, nanotechnology, electronics, and energy research, this book underscores the advantages of MXenes as a versatile platform for next-generation devices, including high-performance sensors, biointegrated systems, energy-efficient computing components, and safe, fast-charging batteries. Written for researchers, graduate students, and professionals, the book provides valuable insights into current challenges and future opportunities, serving as a helpful reference for those seeking to understand and exploit MXenes and related two-dimensional materials in advanced functional applications.

Chonghe Li, Materials Science Series Editor

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