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Recent advances in MXenes: synthesis, properties, applications, and DFT-based investigations

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ABSTRACT: MXenes have emerged as a rapidly growing family of two-dimensional (2D) transition-metal carbides, nitrides, and carbonitrides that exhibit a unique combination of excellent electrical conductivity, large specific surface area, outstanding mechanical properties, and tunable surface chemistry. Since their first discovery in 2011 through the selective etching of MAX phases, MXenes have attracted significant attention from both experimental and theoretical research communities. Their distinctive structural characteristics and versatile physicochemical properties have enabled a wide range of applications in energy storage, gas sensing, flexible electronics, environmental remediation, catalysis, biomedicine, and electromagnetic interference shielding. In particular, the presence of abundant surface functional groups and controllable electronic structures provides exceptional opportunities for tailoring their performance for specific technological applications. This review provides a comprehensive overview of MXenes, including their crystal structures, synthesis methods, fundamental properties, and major technological applications. Various synthesis approaches, ranging from conventional chemical etching to emerging electrochemical and molten-salt methods, are discussed. The outstanding electrical, mechanical, chemical, and optical properties of MXenes are highlighted, with particular emphasis on their structure–property relationships. Furthermore, recent advances in MXene-based applications in energy storage systems, gas sensors, environmental technologies, flexible electronics, and electromagnetic shielding are summarized. In addition, the role of density functional theory (DFT) calculations in understanding and predicting the behavior of MXenes is critically reviewed. Theoretical studies on electronic structure engineering, gas adsorption, atomic doping, ion storage, catalysis, and spintronic applications are discussed to demonstrate the importance of first-principles simulations in guiding experimental developments. Overall, MXenes represent a highly promising class of multifunctional materials with enormous potential for next-generation electronic, energy, environmental, and biomedical technologies.

KEYWORDS: MXenes, two-dimensional materials, energy storage, gas sensing, flexible electronics, environmental remediation, electrocatalysis.

1. INTRODUCTION TO MXenes

MXenes are an emerging family of two-dimensional (2D) nanomaterials that were first discovered in 2011 through the selective exfoliation and etching of layered MAX phases [1]. MAX phases are a class of ternary layered compounds with the general formula Mn+1AXn, where M represents an early transition metal, A is an element from groups IIIA or IVA, and X denotes carbon and/or nitrogen [2]. Owing to their unique layered crystal structure, the A layers can be selectively removed by appropriate chemical etching processes, leading to the formation of a new class of two-dimensional materials known as MXenes. The resulting MXenes possess the general formula Mn+1XnTx, where Tx represents various surface termination groups, such as –O, –OH, –F, and – Cl, which are introduced during the synthesis process and strongly influence the physicochemical properties of the material [2,3]. Since their discovery, MXenes have attracted tremendous attention because they combine the structural advantages of two-dimensional materials with the rich compositional diversity of transition-metal carbides and nitrides. Unlike graphene, which consists solely of carbon atoms, MXenes offer a wide range of tunable electronic, magnetic, optical, and chemical properties through variations in composition, surface functionalization, and structural engineering. Owing to their graphene-like layered morphology, high electrical

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conductivity, large surface area, and exceptional tunability, MXenes have rapidly emerged as one of the most extensively studied classes of two-dimensional materials in modern materials science and nanotechnology [2–4].

2. STRUCTURE AND SYNTHESIS OF MXenes

MXenes are typically synthesized from MAX phases through selective chemical etching processes designed to remove the A-element layer located between the transition-metal and carbon/nitrogen layers [1,2]. MAX phases, which possess the general formula Mn+1AXn, serve as the precursor materials for MXene production due to their unique layered crystal structures, where the A layer is relatively weakly bonded compared with the strong M–X bonds [1,2]. This structural characteristic enables the selective extraction of the A-element layer while preserving the integrity of the transition-metal carbide or nitride framework. The etching process is commonly performed using hydrofluoric acid (HF), which was employed in the first successful synthesis of MXenes, or through safer alternative etching systems such as LiF/HCl mixtures that generate HF in situ and allow better control over the exfoliation process [5]. Following the removal of the A layer, the resulting multilayered MXene structures can be further delaminated into ultrathin two-dimensional nanosheets with thicknesses of only a few atomic layers [5,6]. The delamination process is often facilitated by organic intercalants or alkali metal ions, which increase the interlayer spacing and weaken the van der Waals interactions between adjacent layers. As a result, single-layer or fewlayer MXene nanosheets with high surface areas and excellent dispersibility can be obtained, making them highly attractive for a wide range of technological applications [5,6]. During the synthesis process, the freshly exposed MXene surfaces are typically terminated with various functional groups, including O, OH, and F, which originate from the etching environment. These surface terminations play a critical role in determining the electronic, chemical, optical, and mechanical properties of MXenes by influencing their surface reactivity, electrical conductivity, hydrophilicity, and interfacial interactions with other materials [2,3]. Consequently, controlling the type and concentration of surface functional groups has become an important strategy for tailoring the performance of MXenes for specific applications. In addition to conventional chemical etching methods, considerable efforts have been devoted to developing alternative synthesis approaches that can improve product quality, reduce environmental concerns, and expand the diversity of available MXene compositions [3,6]. These emerging techniques include electrochemical etching, molten-salt etching, hydrothermal synthesis, and bottom-up fabrication strategies. Such approaches offer enhanced control over composition, morphology, defect density, and surface chemistry, thereby enabling the preparation of MXenes with improved structural stability and functional performance. The continuous advancement of synthesis technologies is expected to facilitate the large-scale production of high-quality MXenes and further broaden their applications in energy storage, sensing, catalysis, environmental remediation, and next-generation electronic devices [3,6].

3. FUNDAMENTAL PROPERTIES OF MXenes

MXenes possess a unique combination of outstanding properties that have made them highly attractive for a broad range of scientific and technological applications. One of their most remarkable characteristics is their exceptionally high electrical conductivity, with several MXene compositions exhibiting metallic-like behavior and conductivities reaching tens of thousands of S/cm [2,3]. Such excellent electrical transport properties originate from the metallic nature of many transition-metal carbide and nitride layers, making MXenes promising candidates for applications in energy storage, sensing technologies, and advanced electronic devices [2,3]. In addition, their two-dimensional layered structure provides a large specific surface area, which is highly beneficial for adsorption processes, surface reactions, and charge-transfer phenomena [3,7]. The high surface-to-volume ratio not only increases the number of active sites available for molecular interactions but also facilitates rapid ion diffusion and electron transport, thereby enhancing the performance of MXene-based devices in electrochemical and catalytic applications [3,7]. Furthermore, the interlayer spacing of MXenes can be modified through intercalation or surface engineering, providing additional opportunities for optimizing their physicochemical properties. The presence of surface functional groups further imparts excellent hydrophilicity, enabling easy dispersion in aqueous and polar solvents and facilitating the fabrication of thin films, coatings, membranes, and composite materials [10,11]. Unlike many other two-dimensional materials that suffer from poor dispersibility, MXenes can form stable colloidal suspensions, which greatly simplifies their processing and integration into practical devices. These surface terminations also contribute significantly to the chemical reactivity and tunability of MXenes, allowing their properties to be tailored for specific applications [10,11]. Moreover, MXenes exhibit excellent mechanical strength, structural stability, and flexibility, making them suitable for flexible and wearable electronic systems. Their electronic, optical, and magnetic properties can be effectively tuned through atomic doping, defect engineering, surface functionalization, and compositional modification. Numerous theoretical and experimental studies have demonstrated that such modifications can induce substantial changes in the electronic band structure, magnetic ordering, optical absorption characteristics, and catalytic activity of MXenes, thereby expanding their application potential in nanoelectronics, optoelectronics, spintronics, and energy conversion technologies [8,15]. These unique characteristics provide MXenes with significant advantages over many other two-dimensional materials and contribute to their growing importance in advanced materials research and emerging nanotechnology applications [11,8].

4. APPLICATIONS OF MXenes

Owing to their exceptional physicochemical properties, MXenes have found extensive applications across a wide range of advanced technological fields [3–10]. Their unique combination of high electrical conductivity, large specific surface area, excellent mechanical flexibility, tunable surface chemistry, and superior hydrophilicity has enabled their utilization in numerous emerging technologies, making them one of the most promising families of twodimensional materials for next-generation devices and systems [3–10]. In the area of energy storage, MXenes have been widely employed as electrode materials for lithium-ion, sodium-ion, and potassium-ion batteries, as well as supercapacitors, owing to their high electrical conductivity, large specific surface area, and efficient ion transport characteristics [3,7]. The layered structure of MXenes facilitates rapid ion intercalation and diffusion, while their conductive framework promotes fast electron transport, resulting in enhanced energy-storage performance, high rate capability, and excellent cycling stability [3,7]. Consequently, MXenes have emerged as highly attractive candidates for advanced electrochemical energy-storage technologies. In gas-sensing applications, MXenes exhibit remarkable sensitivity toward various gas molecules, including NH_3, NO_2, CO, and H_2S, primarily due to significant changes in their electronic structure upon gas adsorption on the surface [10,11]. The abundance of active surface sites and functional groups facilitates strong interactions between gas molecules and the MXene surface, leading to measurable variations in electrical conductivity or resistance. These characteristics enable MXenebased sensors to achieve high sensitivity, rapid response and recovery times, and excellent selectivity for environmental monitoring and industrial safety applications [10,11]. For electronic applications, MXenes have been extensively investigated for the fabrication of field-effect transistors, conductive electrodes in flexible electronic devices, transparent conductive films, and printed electronic systems [9,12]. Their outstanding electrical conductivity and mechanical flexibility make them particularly suitable for wearable electronics, flexible displays, and nextgeneration integrated electronic circuits. In addition, MXenes can be readily processed into thin films and inks, facilitating scalable and cost-effective device fabrication [9,12]. In the environmental sector, MXenes demonstrate outstanding adsorption capabilities toward heavymetal ions, organic dyes, radioactive species, and various pollutants, thereby offering promising opportunities for water purification and environmental remediation [10,19]. Their large surface area and abundant surface functional groups provide numerous active sites for contaminant capture and removal. As a result, MXene-based materials have attracted significant attention for wastewater treatment, desalination, and pollutant remediation technologies [10,19]. Furthermore, MXenes have shown great potential in electrocatalysis, photocatalysis, sustainable hydrogen production, biosensing, and drug-delivery systems for biomedical applications [10,14]. Their tunable electronic structures, excellent charge-transfer properties, and versatile surface chemistry make them suitable for a variety of catalytic and biomedical functions. Recent studies have demonstrated that MXene-based nanostructures can significantly enhance catalytic activity and improve the efficiency of energy-conversion processes, while also serving as effective platforms for biosensing and therapeutic applications [10,14]. Notably, owing to their excellent electromagnetic wave absorption and reflection capabilities, MXenes are recognized as one of the most effective materials for electromagnetic interference (EMI) shielding, providing significant opportunities for applications in electronics, telecommunications, aerospace, and defense technologies [13]. Their high electrical conductivity and layered architecture enable efficient attenuation of electromagnetic radiation through multiple reflection, absorption, and scattering mechanisms. Consequently, MXenes have emerged as highly promising materials for protecting sensitive electronic components and ensuring electromagnetic compatibility in modern technological systems [13].

5. MXENES IN DENSITY FUNCTIONAL THEORY (DFT) STUDIES

In addition to experimental investigations, MXenes have attracted considerable attention in computational materials research based on density functional theory (DFT) [15,8]. Owing to their compositional diversity, tunable surface chemistry, and unique electronic characteristics, MXenes have emerged as an ideal platform for theoretical studies aimed at understanding and predicting structure–property relationships at the atomic scale. DFT calculations provide valuable insights into the fundamental mechanisms governing the electronic, magnetic, optical, and catalytic behaviors of MXenes, thereby complementing experimental observations and facilitating the rational design of novel MXene-based materials [15,8]. Theoretical studies have demonstrated that MXenes possess rich and versatile electronic structures that can be effectively tuned through molecular adsorption, atomic doping, and surface functionalization [8,7]. Depending on their chemical composition and surface terminations, MXenes may exhibit metallic, semiconducting, or even magnetic characteristics, making them highly attractive for a variety of electronic and energy-related applications. Furthermore, the strong dependence of their electronic properties on surface chemistry provides an effective strategy for tailoring material performance through controlled modification of the atomic structure [8,7]. Numerous studies have explored the adsorption behavior of gas molecules, including CO, NO_2, NH_3, and SO_2, on various MXene systems to evaluate their potential applications in gas-sensing technologies [17,16]. These investigations have revealed strong interactions between gas molecules and MXene surfaces, often accompanied by significant charge transfer and noticeable changes in the electronic structure. Such effects can lead to measurable variations in conductivity, magnetic moments, or work functions, thereby enabling the development of highly sensitive and selective gas sensors. Theoretical calculations have also provided important insights into adsorption energies, charge-transfer mechanisms, and recovery characteristics that are difficult to obtain solely through experimental approaches [17,16]. Furthermore, the incorporation of transition-metal dopants such as Fe, Co, Ni, and Mn has been shown to significantly modify the electronic band structure and magnetic properties of MXenes [7,17]. Atomic doping can induce magnetism, alter carrier concentrations, create localized electronic states, and improve catalytic activity. These modifications offer effective routes for tailoring MXene properties to meet the requirements of specific applications in nanoelectronics, spintronics, and energy conversion technologies. In particular, several theoretical studies have predicted the emergence of half-metallic behavior and enhanced magnetic ordering in doped MXene systems, highlighting their potential for spin-dependent electronic devices [7,17]. Beyond gas sensing, DFT investigations have also focused extensively on metalion storage capabilities, optical properties, electrocatalytic performance, and spintronic applications [15,7]. Computational studies have been widely employed to evaluate ion adsorption energies, diffusion barriers, electronic conductivity, and reaction pathways in MXene-based electrode materials, providing valuable guidance for the development of high-performance batteries and supercapacitors. Similarly, DFT calculations have contributed significantly to understanding light–matter interactions, catalytic reaction mechanisms, and spin-polarized electronic transport in various MXene systems [15,7]. These findings highlight the great promise of MXenes as a versatile materials platform for the design and development of next-generation electronic and energy-related devices and demonstrate the crucial role of first-principles simulations in accelerating MXene research and technological innovation.

6. CONCLUSIONS

MXenes constitute an advanced family of two-dimensional (2D) materials that uniquely combine high electrical conductivity, large specific surface area, excellent hydrophilicity, superior mechanical robustness, and tunable physical properties through compositional modification and surface functionalization. These outstanding characteristics have established MXenes as one of the most intensively investigated material platforms in contemporary materials science. Owing to their broad application potential in energy storage, sensing technologies, flexible electronics, environmental remediation, catalysis, biomedicine, and electromagnetic interference (EMI) shielding, MXenes are expected to play a pivotal role in the development of next-generation advanced technologies. Furthermore, density functional theory (DFT)-based computational studies continue to provide fundamental insights into the underlying mechanisms governing the structural, electronic, magnetic, and chemical properties of MXenes, thereby facilitating the rational design and optimization of MXene-based systems for a wide range of practical applications.

REFERENCES

1. Naguib, M., Kurtoglu, M., Presser, V., Lu, J., Niu, J., Heon, M., Hultman, L., Gogotsi, Y., & Barsoum, M. W. (2011). Two-dimensional nanocrystals produced by exfoliation of Ti_3AlC_2. *Advanced Materials, 23*(37), 4248–4253. https://doi.org/10.1002/adma.201102306
2. Naguib, M., Mochalin, V. N., Barsoum, M. W., & Gogotsi, Y. (2014). 25th anniversary article: MXenes: A new family of two-dimensional materials. *Advanced Materials, 26*(7), 992–1005. https://doi.org/10.1002/adma.201304138
3. Anasori, B., Lukatskaya, M. R., & Gogotsi, Y. (2017). 2D metal carbides and nitrides (MXenes) for energy storage. *Nature Reviews Materials, 2*, Article 16098. https://doi.org/10.1038/natrevmats.2016.98
4. Anasori, B., & Gogotsi, Y. (Eds.). (2019). *MXenes: Synthesis, properties and applications*. Springer Nature. https://doi.org/10.1007/978-3-030-19026-3
5. Ghidiu, M., Lukatskaya, M. R., Zhao, M. Q., Gogotsi, Y., & Barsoum, M. W. (2014). Conductive two-dimensional titanium carbide "clay" with high volumetric capacitance. *Nature*, *516*, 78–81. https://doi.org/10.1038/nature13970
6. Alhabeb, M., Maleski, K., Anasori, B., Lelyukh, P., Clark, L., Sin, S., & Gogotsi, Y. (2017). Guidelines for synthesis and processing of two-dimensional titanium carbide ($Ti_3C_2T_x$ MXene). *Chemistry of Materials, 29*(18), 7633–7644. https://doi.org/10.1021/acs.chemmater.7b02847
7. Xie, Y., Dall'Agnese, Y., Naguib, M., Gogotsi, Y., Barsoum, M. W., Zhuang, H. L., & Kent, P. R. C. (2014). Prediction and characterization of MXene nanosheet anodes for non-lithium-ion batteries. *ACS Nano, 8*(9), 9606–9615. https://doi.org/10.1021/nn503921j
8. Khazaei, M., Arai, M., Sasaki, T., Chung, C. Y., Venkataramanan, N. S., Estili, M., Sakka, Y., & Kawazoe, Y. (2013). Novel electronic and magnetic properties of twodimensional transition metal carbides and nitrides. *Advanced Functional Materials, 23*(17), 2185–2192. https://doi.org/10.1002/adfm.201202502
9. Zhang, C., McKeon, L., Kremer, M. P., et al. (2019). Additive-free MXene inks and direct printing of micro-supercapacitors. *Nature Communications, 10*, Article 1795. https://doi.org/10.1038/s41467-019-09398-1

10. Rasool, K., Pandey, R. P., Rasheed, P. A., Buczek, S., Gogotsi, Y., & Mahmoud, K. A. (2019). Water treatment and environmental remediation applications of two-dimensional metal carbides (MXenes). *Materials Today*, *30*, 80–102. https://doi.org/10.1016/j.mattod.2019.05.017
11. Lee, E., VahidMohammadi, A., Yoon, Y. S., Beidaghi, M., & Kim, D. J. (2017). Twodimensional vanadium carbide MXene for gas sensors with ultrahigh sensitivity toward ammonia. *ACS Sensors*, *2*(10), 1415–1422. https://doi.org/10.1021/acssensors.7b00466
12. Aghamohammadi, H., Tavakoli, O., et al. (2022). MXene-based flexible electronics: A review. *Nano-Micro Letters, 14*, Article 161. https://doi.org/10.1007/s40820-022-009087
13. Shahzad, F., Alhabeb, M., Hatter, C. B., Anasori, B., Hong, S. M., Koo, C. M., & Gogotsi, Y. (2016). Electromagnetic interference shielding with 2D transition metal carbides (MXenes). *Science*, *353*(6304), 1137–1140. https://doi.org/10.1126/science.aag2421
14. Lin, H., Wang, X., Yu, L., Chen, Y., & Shi, J. (2017). Two-dimensional ultrathin MXene ceramic nanosheets for photothermal conversion. *Advanced Materials, 29*(4), Article 1603942. https://doi.org/10.1002/adma.201603942
15. Khazaei, M., Ranjbar, A., Arai, M., Sasaki, T., & Yunoki, S. (2017). Electronic properties and applications of MXenes: A theoretical review. *Journal of Materials Chemistry C, 5*(10), 2488–2503. https://doi.org/10.1039/C6TC05264F
16. Shuck, C. E., & Gogotsi, Y. (2020). MXene-based gas sensors. *ACS Nano*, *14*(8), 9692– 9710. https://doi.org/10.1021/acsnano.0c05684
17. Zhou, J., & Sun, Z. (2015). Half-metallic ferromagnetism and surface functionalizationinduced metal–insulator transition in graphene-like two-dimensional Cr_2C crystals. *ACS Applied Materials & Interfaces*, *7*(31), 17510–17515. https://doi.org/10.1021/acsami.5b04091