

Transition Metal Carbide and Nitride Composite Nanoarchitectonics for Bio-, Electro-, and Photo-Based Catalytic Applications

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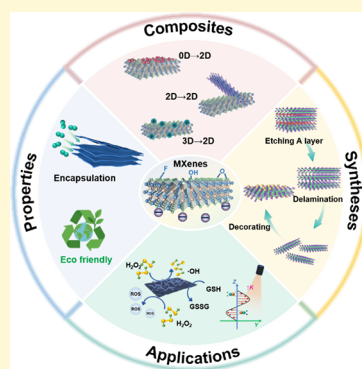


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ABSTRACT: MXenes have emerged as a versatile two-dimensional platform in advanced catalytic systems because of their tunable surface chemistry, metallic conductivity, and structural diversity. Nevertheless, severe agglomeration and limited colloidal stability may undermine their catalytic performance. Integrating MXenes with low-dimensional materials through rational nanoscale construction mitigates these limitations while enhancing mass and charge transport, interfacial performance, dispersion, and catalytic activity. This review focuses on the design, functionality, and catalytic applications of MXene-based composites. It begins with a brief introduction to the chemical and crystal structures of MAX phases and MXenes, followed by an overview of representative MXene-based composites, including 0D–2D, 2D–2D, and 3D–2D systems. The article then discusses their applications in heterogeneous catalysis, photocatalysis, biocatalysis, and electrocatalysis. Finally, we summarize the perspectives, highlighting the current challenges and future opportunities in the rational design and industrial transformation of MXene composite nanoscale construction.



Catalysis plays an indispensable role in sustainable chemical manufacturing, environmental remediation, energy conversion, and biomedical applications by enabling efficient and selective chemical transformations.¹ The increasing demand for high-performance catalytic systems has driven the rational design of advanced catalysts with improved activity, selectivity, and long-term stability.² In particular, nanostructured catalysts have attracted considerable attention because of their tunable physicochemical properties, abundant active sites, and controllable architectures, offering unique opportunities to steer catalytic processes toward sustainable technologies.³

Recent advances in nanotechnology have enabled the rational design of nanostructured catalysts with controllable compositions, interfaces, and architectures for diverse catalytic applications.^{4,5} Beyond the intrinsic properties of individual nanomaterials, increasing attention has focused on how nanoarchitectural organization collectively regulates catalytic performance. Guided by the concept of nanoarchitectonics, the rational integration of nano-building blocks, interfaces, and hierarchical architectures has emerged as an effective strategy for creating functions beyond those of the individual components.^{6–8} Among the diverse nanomaterial platforms investigated to date, two-dimensional (2D) materials are particularly attractive because of their ultrathin architectures, accessible surfaces, and tunable electronic structures, making them promising candidates for catalytic applications.^{7,9,10} Crucially, recent research in nanoarchitectonics highlights that catalytic performance depends not only on the intrinsic properties of

nanomaterials, but also on the rational combination of nano-building blocks, interfaces, and hierarchical architectures. These attributes provide a practical framework for developing advanced catalysts using various 2D materials.

Over the past two decades, exploring the physicochemical characteristics of single-layer graphene has led to the discovery of diverse 2D materials, including metal dichalcogenides (TMDCs) and boron nitride.^{11,12} Due to their ultrathin architecture, tunable electronic structure, and abundant surface atoms, these 2D materials have attracted considerable interest for catalytic applications.¹³ Among the vast family of 2D materials, MXenes (pronounced “max-enes”) are a rapidly expanding family of transition metal carbides, nitrides, and carbonitrides derived from parent MAX phases.¹¹ Since their advent in 2011, extensive studies have resulted in the generation of MAX phases (over 150 kinds) and their MXene derivatives (over 30) with varying compositions, exhibiting remarkable physicochemical characteristics, including high electrical conductivity ($\sim 24,000$ S/cm), abundant surface chemistry, tunable electronic structures, and structural versatility.^{11,13,14} Compared

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with other representative 2D materials, such as graphene, hexagonal boron nitride, and TMDCs, MXenes possess several unique characteristics that make them particularly attractive catalytic platforms.^{15,16} Firstly, the abundant surface terminations ($-O$, $-OH$, and $-F$) facilitate the immobilization of catalytically active species and strengthen interfacial interactions with reactants.¹⁷ The 2D lamellar architecture provides a large specific surface area with abundant exposed active sites, while the intrinsic metallic conductivity promotes rapid electron transport and accelerates catalytic kinetics.¹⁸ Furthermore, the excellent hydrophilicity improves wettability and reactant diffusion, making MXenes especially suitable for aqueous catalytic systems.¹⁹

Despite these remarkable advantages, pristine MXenes still suffer from several intrinsic limitations, particularly restacking, aggregation, and limited colloidal stability caused by strong van der Waals interactions between adjacent nanosheets. These issues reduce accessibility, hinder mass transport, and ultimately compromise catalytic performance.²⁰ To overcome these limitations, nanoarchitected MXene composites have been extensively developed through their integration with various low-dimensional (0–2D) materials. Such rational nanoarchitectonics not only reduces aggregation and improves structural stability but also tailors interfacial interactions, electronic structures, and surface characteristics, thereby enhancing mass/electron transfer, exposing more catalytically active sites, and generating synergistic catalytic effects.^{20,21} Rather than representing a simple combination of different components, such nanoarchitectures embody the concept of nanoarchitectonics, emphasizing the deliberate integration of nanoscale building

blocks through interface engineering and hierarchical structural regulation to establish desired structure-property-function relationships.^{22,23}

Building on this nanoarchitectonics concept, MXene composites have attracted increasing interest in various kinds of catalytic applications. Although reviews on MXenes have recently been published, most focus on synthesis,²⁴ properties,^{25,26} a single composite,^{27,28} and a single application, including photocatalysis,^{29,30} and electrocatalysis,^{31,32} as well as their combination.^{16,33–36} Moreover, an integrated perspective that systematically correlates nanoarchitectural design of composites and their multifunctional catalytic performance across diverse catalytic systems is still insufficiently documented. From a nanoarchitectonics perspective, MXene composite nanoarchitectonics has emerged as a versatile catalytic platform, in which rational nanoarchitectural design and interface engineering collectively regulate the structure–property–function relationship and ultimately govern catalytic performance across various catalytic fields. Accordingly, this review provides a nanoarchitectonics-inspired perspective on MXene composite nanoarchitectonics for catalytic applications. Beginning with the chemistry and crystal structures of MAX phases and MXenes, we discuss synthetic strategies for constructing diverse nanoarchitected composites, followed by an analysis of structure–property relationships that govern catalytic functionality. Finally, we comprehensively summarize representative applications in heterogeneous catalysis, photocatalysis, electrocatalysis, and biocatalysis, along with current challenges and future opportunities for industrial translation (Figure 1).

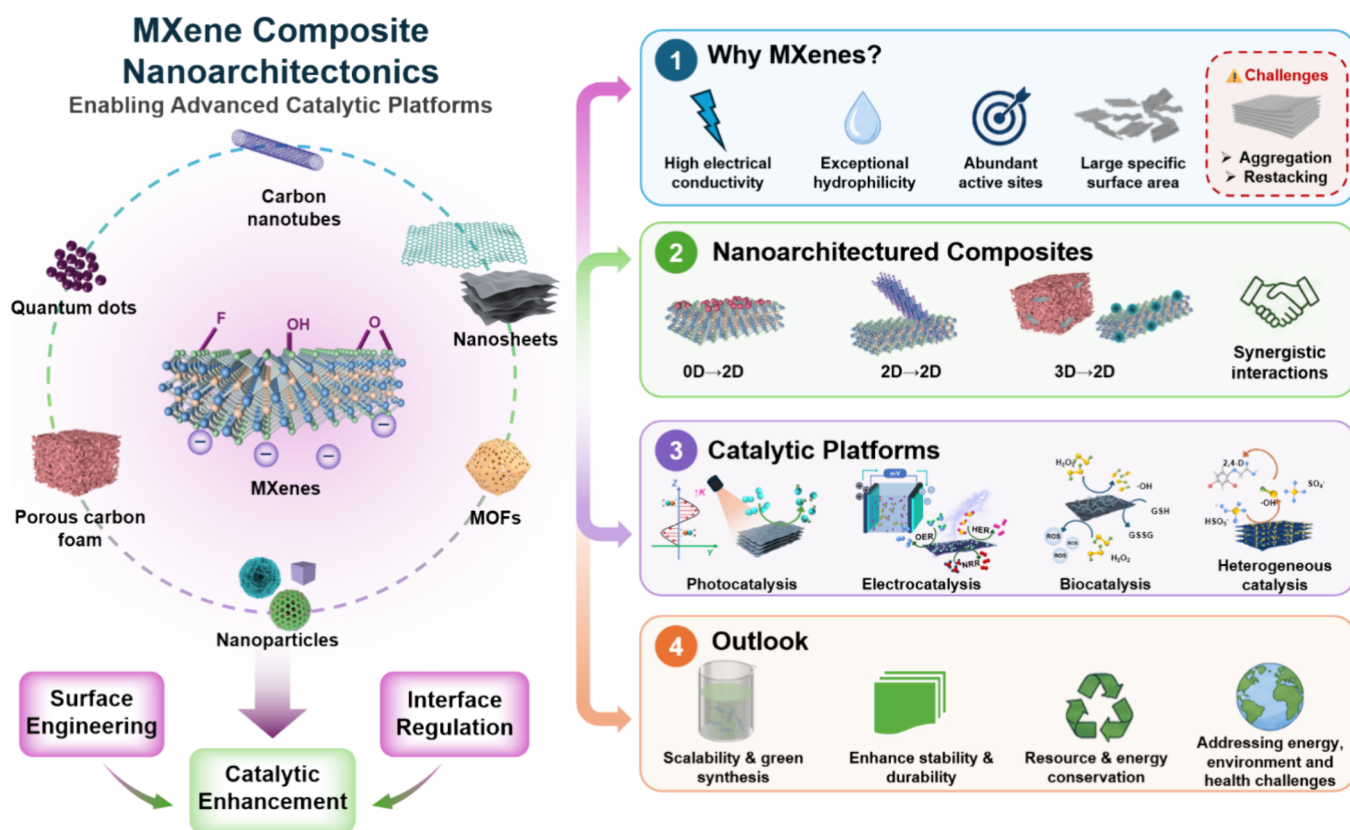


Figure 1. Schematic illustration of nanoarchitected MXene-based composites with various dimensional materials for fabricating advanced catalytic platforms, highlighting their design strategies, interesting synergistic properties, catalytic applications, and prospects.

Among the vast family of 2D materials, MXenes have emerged as one of the most promising classes of materials composed of transition-metal carbides, nitrides, or carbonitrides. Since their advent in 2011, the past decade has evidenced the development of various MAX phases (over 150 kinds) and their MXene derivatives (more than 30), establishing the complete chemistry and configuration of these phases, as well as their derived materials. Establishing the complete chemistry, the generalized structure of MAX phases is presented as $M_{n+1}AX_n$, while MXenes are expressed as $M_{n+1}X_nT_x$ ($n = 1-4$).³⁷ Herein, M indicates an early transition metal species; A represents a group IIIA or IVA element; X represents carbon or nitrogen; T_x refers to various surface terminal groups (typically anions) (Figure 2). Typically, MXenes ($M_{n+1}X_nT_x$) are arranged in such a way that $n + 1$ layers of early transition metals, including scandium (Sc), titanium (Ti), molybdenum (Mo), vanadium (V), niobium (Nb), zirconium (Zr), chromium (Cr), hafnium (Hf), and tantalum (Ta), are enclosed with n layers of X elements (C or N). The terminal surface groups (T_x) are coordinated with the M layers, such as oxy ($-O$), hydroxy ($-OH$), fluoro ($-F$), and/or chloro ($-Cl$). The exceptional architecture of MXenes, formed by transition metals and carbon or nitrogen atoms with surface functional groups, resembles a “brick wall” with significantly tunable physicochemical properties. The major difference between precursor MAX and derivative MXenes lies in the layer architecture: encapsulated Group A elements (groups 13–16) in MAX phases vs MXenes.¹¹ Structurally, the MAX phase is a layered hexagonal crystal structure, with alternating A layers sandwiched between M and X layers. Due to weaker bonds than the covalent/metallic bonds between M and X, the A-layer in the three-dimensional (3D) nano-laminated ceramic MAX precursors is selectively etched with hydrofluoric acid (HF), yielding 2D MXene derivatives with limited layers and various surface functional groups.¹¹ Although MAX phases offer exceptional thermal conductivity and mechanical strength, the derived MXenes provide better surface chemistry, enhanced hydrophilicity, and excellent electrical/ionic conductivity for catalysis and energy storage.³⁷

Considering the structure, the inimitable properties of MXenes arise from metallic/covalent bonds in their lamellar structure, along with the relatively fragile linkages between the layers (M and A). In addition, oxygenated terminal groups preserve conductivity in polar solvents, supporting their use in catalysis. These surface groups play a critical role in tuning electronic properties and influencing interfacial bonding with other 2D materials. When integrated with semiconductors such as graphitic carbon nitride ($g-C_3N_4$), Bi_2WO_6 , or MoS_2 , MXenes enhance electron extraction, promote interfacial charge separation, and increase catalytic reaction rates. The anisotropic carrier (electron and hole) mobility in MXene systems promotes separation of photo-generated electron-hole pairs, making them favorable for photocatalytic hydrogen production and pollutant degradation.³⁸ Furthermore, their excellent chemical stability and hydrophilicity enable superior dispersion in aqueous environments, a feature particularly beneficial for environmental and energy applications.³⁹

The development of MXene-based nanocomposites is typically attributed to active surface functional groups ($-F$, $-OH$, or $-O$), which provide natural binding sites for supramolecules (polymers) and the direct growth of other nanostructures (zero-dimensional, 0D). To modify the surface, the functionalization of MXenes involves establishing either covalent (Ti–O–Si, Ti–O–C, and Ti–O–P) or non-covalent (van der Waals forces and hydrogen bonding) linkages. These surface-alterable linkages on MXenes not only regulate the physicochemical properties but also optimize the oxidation stability and dispersibility. In comparison, non-covalent linkages may be weaker, resulting in lower stability than covalent bonding with MXenes, and *vice versa*. Considering the pros and cons, it is necessary to select the most suitable modification. To this end, 0D (metallic nanoparticles, metal oxides, and magnetic constructs) nanodots (NDs) are often “grown” on the surface or interlayer of MXene using co-precipitation or solution chemical reduction methods, with the key being the nucleation mechanism between the terminating groups on the MXene surface and the NDs precursor in solution. By adjusting concentration,

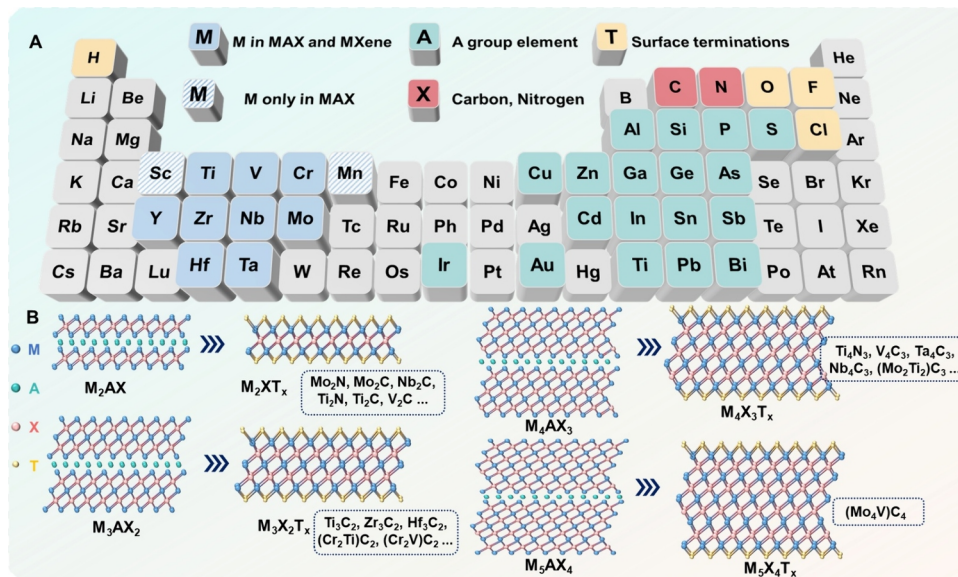


Figure 2. Schematics of the chemical structures of the elements (A) in designed diverse MXenes, accompanied by molecular models and configurations (B).

temperature, reducing agent, or pH, metal ions nucleate and grow into NDs at these sites. In addition, these NDs can be incorporated into MXene interlayers, increasing the spacing between MXene multilayers and facilitating MXene delamination. The intercalation approach not only increases the composite's specific surface area but also improves its electronic transport performance.⁴⁰ In 0D-based composites of MXenes, the main surface bonding modes are coordination bonds (coordination bonding between metal ions and terminating groups), electrostatic interactions, and van der Waals forces.⁴⁰ Similarly, various composite/heterostructures of other 2D materials, such as graphene (GO) and TMDCs, can be stacked with MXenes via simple planar, normal van der Waals forces.⁴¹ Interactions between MXenes and these materials are usually non-covalent, including π - π interactions. Compared with individual MXenes, these hybrid composites further enhance overall properties, including mechanical stability and charge/ion transport ability.

Typically, MXenes are synthesized through chemical etching of MAX phases using HF or *in situ* generated HF (via LiF and HCl mixture). The choice of etching reagent, reaction temperature, and post-treatment strongly influences the surface terminations and morphology of the obtained MXenes.⁴² Subsequent delamination produces few- or single-layer nanosheets (NSs) with accessible surfaces, providing suitable building blocks for composite construction. To prepare MXene-based composites using such precursors and modifications, researchers have employed several strategies, including electrostatic self-assembly,⁴³ hydrothermal/solvothermal methods,^{44,45} calcination,⁴⁶ *in situ* growth/redox deposition,⁴⁷ covalent grafting,⁴⁸ and physical methods (electrospinning, mechanical blending, freeze-drying, and electrophoretic deposition).⁴⁹ Using such methods, we present an overview of various composites, including metal-doped 2D MXene layers, 0D/1D structures-decorated 2D MXene layers, 2D–2D van der Waals heterojunctions, and 2D–3D architectures: frameworks and macrostructures.

■ METAL-DOPED 2D MXENE LAYERS

Altering inorganic frameworks has emerged as an innovative approach to modify their physicochemical characteristics, including their intrinsic stability. Doping of various metals can be achieved either by donating electrons via surface-functionalized molecules or by substituting metals into the framework lattice.⁵⁰ Nevertheless, fabricated metal-doped constructs often yield oxide forms of the guest species, distorting the host framework.² This approach significantly improves the host framework, offering a paradigm for theoretical and experimental investigations. In catalysis, incorporating metal species increases the number of active catalytic sites. Among various metals and non-metals, metal-doped MXenes show improved properties because of their intrinsic participation in various functionalities.⁵¹ You and colleagues doped various transition metals (Cr, Mo, and W) into MXene (Nb_2CO_2) NSs to evaluate their properties using DFT calculations and to explore their performance in gas-sensing applications.⁵² Among them, W-doped Nb_2CO_2 composites exhibited superior performance for H_2 sensing at room temperature. In addition, Mo-doped MXenes emerged as an optimal candidate for H_2S gas sensing. In another case, late transition metal-doped MXenes (Ni-doped $\text{Sc}_3\text{N}_2\text{O}_2$ and Ni-doped $\text{Nb}_3\text{C}_2\text{O}_2$) presented excellent bifunctional electrocatalytic activities for water

splitting reactions towards Hydrogen Evolution Reaction (HER)/Oxygen Evolution Reaction (OER) activities.⁵³ Interestingly, first-principles calculations were combined with machine learning to demonstrate that transition-metal doping promotes HER/OER activity.

■ 0D/1D STRUCTURES-DECORATED 2D MXENE LAYERS

Integrating 0D NDs (SnO_2 , CdS, MoS_2 , Pt, Pt-Ir, TiO_2 , and CeO_2) onto 2D MXenes creates a hierarchical system that merges discrete catalytic activation with continuous charge transport.^{19,54} The designed architecture strategically utilizes the MXene as a conductive, mechanically stable platform to host and electronically communicate with highly active nanoclusters, preventing agglomeration while maximizing exposed active sites. A prominent example of a 0D–2D hierarchical architecture is the anchoring of nickel-doped ceria nanoparticles (Figure 3A).⁵⁴ Isotropic CeO_2 particles, typically below 20 nm (Figure 3B), offer a high surface-to-volume ratio and the potential for quantum confinement effects to degrade pharmaceutical pollutants. The uniqueness lies in the MXene substrate acting as an electron sink, rapidly accepting photogenerated electrons from the semiconductor nanoparticles, thereby drastically prolonging the lifetime of the charge-separated state for catalysis.⁵⁴ The coordination prevents nanoparticle agglomeration and maximizes catalytic exposure, ideal for OER and related redox reactions. The performance of these 0D–2D composite materials stems from powerful electronic interactions at their interface, which actively reshape the local chemical landscape. The spectroscopy reveals that electron flow from the MXene substrate to the anchored nanoparticles directly influences the d-band configuration of the metal catalytic sites. This phenomenon is clearly demonstrated in systems such as Pt NDs on TiO_2 nanowire/ Ti_3C_2 MXene heterostructures for CO_2 reduction.⁵⁵ Figure 3C–F provide direct visual evidence of the 0D (Pt NDs), one-dimensional (1D TiO_2), and 2D (MXenes) components forming an intimate heterostructure, demonstrating the uniform distribution of Pt NDs, addressing agglomeration, and showing electron-conduction bridges. The shift in electron density fine-tunes the binding strength of critical reaction species, such as the $^*\text{OOH}$ intermediate in oxygen reduction, thereby lowering the reaction's energy barrier. Beyond metal oxide-based nanoparticles, researchers have successfully integrated various 0D materials with MXenes, including metal nanoparticles (e.g., Pd, CdS, and MoS_2), imparting unique catalytic, optical, or electronic properties to hybrid composites.¹⁹

■ 2D–2D VAN DER WAALS HETEROJUNCTIONS

The 2D–2D materials stacked through van der Waals heterojunctions have attracted significant attention because of their atomically thin morphology, high surface-to-volume ratio, tunable electronic structure, and mechanical flexibility. These composites offer unique interfacial features and avoid lattice-mismatch issues, facilitating efficient charge transfer, enabling separation, and providing robust structural stability.⁵⁷ The tunable interlayer coupling offers a powerful means to engineer optoelectronic properties for applications in catalysis, electronics, and sensing. The 2D–2D architectures integrate materials such as TMDCs, $g\text{-C}_3\text{N}_4$, black phosphorus, and MXenes.⁵⁸ Incorporating metallic MXenes with semiconducting 2D

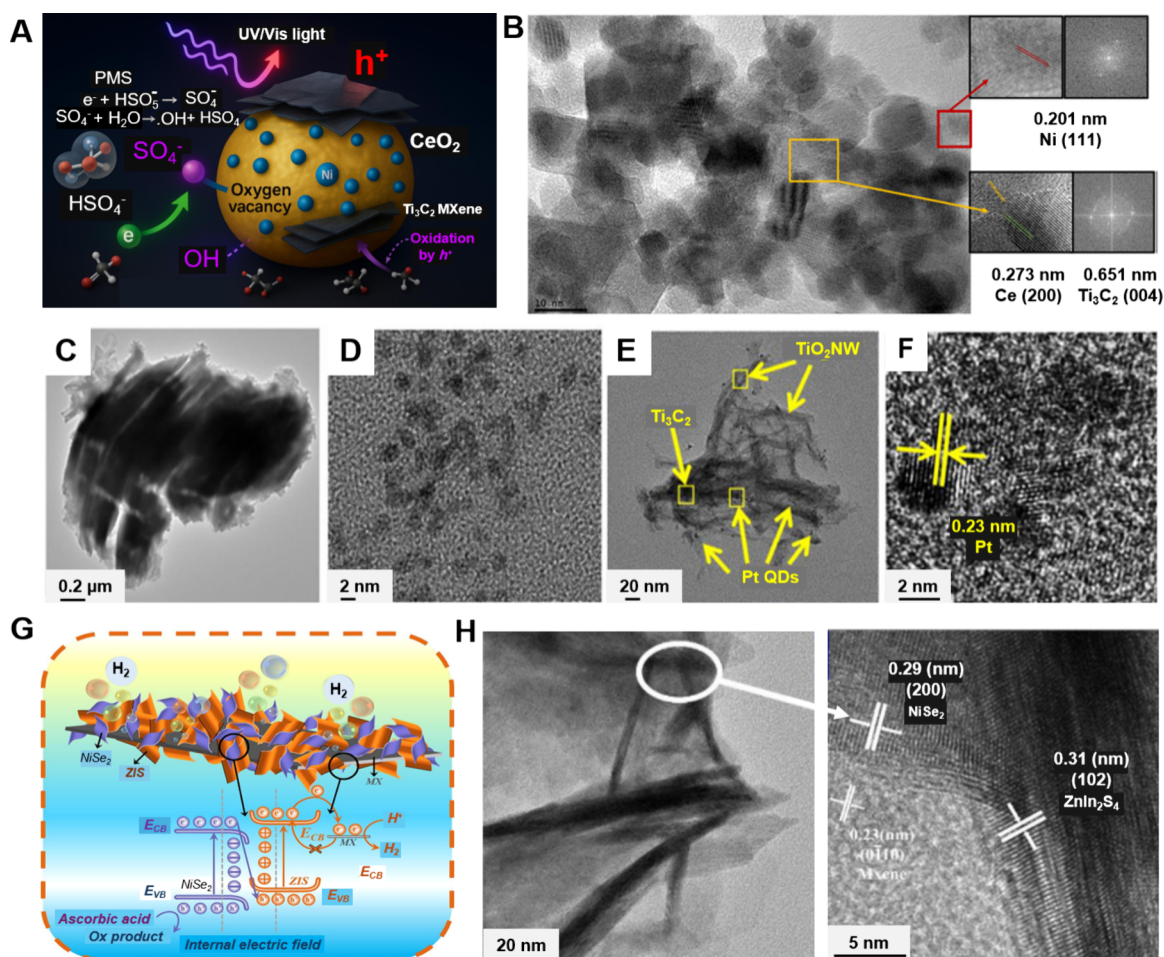


Figure 3. Representative MXene-based multicomponent catalytic heterostructures. (A) Schematic illustrating a 0D-2D hierarchical architecture of transition metal-doped ceria nanoparticles anchored on $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes. (B) HR-TEM image of Ni-doped CeO_2 nanoparticles integrated with $\text{Ti}_3\text{C}_2\text{T}_x$ MXene, illustrating a tight 0D-2D interface for enhanced charge transfer. Reproduced with permission from ref 54 Copyright 2025, Elsevier. (C–F) TEM and HR-TEM images of the 0D/1D-2D Pt- $\text{TiO}_2\text{NW}/\text{Ti}_3\text{C}_2$ heterostructure, showing Pt NDs (circled) anchored on the scaffold. Reproduced with permission from ref 55 Copyright 2023, Elsevier. (G) Schematic diagram of the fabrication of Ti_3C_2 - ZnIn_2S_4 - NiSe_2 composites. (H) Representative TEM and HR-TEM images of MX-ZIS- NiSe_2 , showing its heterostructured morphology and local lattice features. Reproduced with permission from ref 56 Copyright 2022, Elsevier.

materials not only provides a conductive channel for electron transport but can also efficiently harvest solar energy to drive redox reactions.⁵⁹ Enhanced light absorption, efficient charge separation, and prolonged carrier lifetimes are crucial factors for improving photocatalytic and electrocatalytic performance. During the alignment of two different 2D materials with varied functionalities, electrons flow from the lower-efficiency material to the higher-efficiency one until Fermi-level equilibrium is established. The strength and direction of this internal field can be tuned by selecting materials with appropriate band structures and modifying their surface functional groups. Different heterojunction configurations can be fabricated by tuning band alignment and relative energy levels. In type-I alignment, both the conduction and valence bands of one semiconductor lie within those of the other, leading to confinement of charge carriers in one layer. In type-II systems, the conduction and valence bands of the two materials are staggered, allowing electrons and holes to separate into distinct layers. Recently, advanced charge-transfer mechanisms, such as Z-scheme and S-scheme heterojunctions, have been introduced to describe

systems that preserve strong redox potentials while maintaining efficient charge transport.⁶⁰ In S-scheme heterojunctions, photogenerated electrons of one semiconductor recombine with holes in the valence band of another, leaving behind high-energy electrons and holes with strong reducing and oxidizing abilities (Figure 3G,H).⁵⁶

Though highly promising, MXenes are prone to surface oxidation after exposure to air or moisture, which degrades their conductivity and catalytic activity. In addition to protection, the van der Waals assembly of MXenes with other layered structures, such as $g\text{-C}_3\text{N}_4$ or TMDCs, provides a considerably powerful route to precisely tailor internal electric fields and control band alignment at the interface. The catalytic efficacy of these heterojunctions is highly sensitive to the stacking angle and interlayer distance, which dictate electronic-wavefunction overlap and the strength of interfacial coupling. Recent work on a twisted MXene/ MoS_2 bilayer revealed that a specific moiré superlattice periodicity could create localized regions of enhanced charge density that act as catalytic “hot spots”. The performance of 2D–2D heterojunctions is not solely

determined by the individual materials but largely by the interfacial structure and morphology.⁶¹ For photocatalytic and electrocatalytic applications, heterojunction efficiency is often evaluated by its ability to promote redox reactions, such as HER/OER or CO₂ reduction. In photocatalytic HER, for example, van der Waals heterostructures facilitate efficient charge transfer between the light-absorbing semiconductor and the conductive partner material.⁶² In electrocatalysis, 2D–2D heterostructures enhance catalyst activity by modulating the electronic structure at the interface. Combining metallic and semiconducting components optimizes adsorption energies for reaction intermediates, lowering the activation energy for key steps in reactions such as HER/OER and nitrogen fixation.⁶³ Environmental remediation represents another domain for 2D–2D van der Waals heterojunctions. Enhanced separation of photogenerated carriers within these structures facilitates the degradation of organic pollutants such as dyes, antibiotics, and pesticides.⁴³ Despite these advances, several challenges remain, including the scalable synthesis of uniform, defect-free heterostructures, charge-transport hindrance due to uncontrolled stacking orientations, and the introduction of recombination centers. Additionally, understanding charge-transfer processes at the atomic scale remains a formidable task. While theoretical studies have provided valuable insights, directly visualizing interfacial charge dynamics requires advanced techniques such as ultrafast transient absorption spectroscopy, in situ transmission electron microscopy, and Kelvin probe force microscopy. Addressing these challenges will require a synergistic approach that combines experimental innovations with computational modeling.⁶⁴

■ 2D–3D ARCHITECTURES: FRAMEWORKS AND MACROSTRUCTURES

Architectural design, achieved by assembling MXene NSs, alone or in combination, into 3D monoliths (aerogels and foams), marks a critical advancement in their application and effectively overcomes restacking in their 2D forms.^{65,66} This strategic architectural shift goes beyond simple morphological control by engineering a hierarchical porous network, imbuing the material with enhanced mechanical integrity and synergistic interactions among its components.⁶⁷ Evidently, these tailored 3D frameworks could be highly effective in domains such as electrocatalysis and flexible electronics, functioning as active, versatile components integral to device performance.⁶⁸ Recently, a study illustrated the principle by designing a 3D N-doped graphene/MXene (MXene/NGA) aerogel for the oxygen reduction reaction (ORR).⁶⁹ The hydrothermal co-assembly and freeze-drying synthesis creates an interconnected macro-mesoporous network that effectively prevents restacking of both MXene and graphene sheets. The resultant hybrid aerogel exhibited a remarkably high specific surface area of 790 m²/g and a pore size distribution of 12–100 nm, ideal for electrolyte permeation and O₂ diffusion. This hierarchical porous network interaction optimizes the electronic structure of the catalytic sites, facilitating the rate-determining step in ORR. In another instance, a compressible MXene/N-doped Carbon Foam (MXene/NCF) was developed for flexible electronic applications, demonstrating endurance to repeated bending and compression (Figure 4A,B).⁶⁵ The fascinating 3D architecture features interconnected hollow structures, with an MXene layer serving as a continuous, highly conductive sheath. A 3D

MXene/graphene oxide hybrid aerogel demonstrated superior performance in capacitive deionization and electrocatalytic sensing.⁶⁶

■ STRUCTURE-PROPERTY RELATIONSHIPS: FROM ARCHITECTURE TO FUNCTION

The transition of MXenes from promising materials to elite catalysts hinges on a fundamental shift from unexpected discovery materials to rational design. This paradigm is governed by definitive structure-property associations, in which hierarchical architectural parameters spanning the sub-nanometer interlayer gap to the macroscopic pore network directly control catalytic output. Typically, the interlayer distance (d-spacing) in the van der Waals gap between adjacent MXene sheets represents a confined nanofluidic channel that critically governs ion solvation structure and mobility. An optimal d-spacing sterically hinders ion hydration shell formation, creating a high-energy barrier to diffusion. Conversely, an excessively wide energy gap weakens electronic coupling across the layers, enhances permeability, and impairs the continuous supply of electrons to the catalytic interface.⁷⁰ The meticulously designed multi-scale architecture, with electronic-structure modulation and interfacial synergism, intrinsically governs the functional performance of MXene-based materials.¹⁷

Biocatalysis, a fundamental concept in bioengineering, refers to using biological systems to catalyze the regio- and/or stereospecific conversion of (bio)chemicals, including cellular extracts or specific enzymes. MXenes can be used as biocatalysts for biosensing because of their highly electroactive functionalities. Before exploring MXenes' functionality in biocatalysis, it is imperative to understand the cellular balance between oxidative and antioxidant systems. In response to external stimuli, disruption of this redox balance results in excessive ROS production, leading to oxidative damage and contributing to various oxidative stress-related diseases.^{72,73} MXene NSs present a distinctive feature of free radical scavenging through redox reactions, including ROS and reactive nitrogen species (RNS), such as hydroxyl ([•]OH), superoxide (O₂^{•-}), 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) radicals (ABTS⁺), and 1,1-diphenyl-2-picrylhydrazyl radical (DPPH[•]). MXenes with a lamellar structure and alternating weak van der Waals forces can act as intermediates, accelerating reaction rates in biocatalysis (Table 1). Liu and colleagues demonstrated the mechanism through the reaction between Ti₃C₂T_x and H₂O₂, which they used to design a colorimetric strip assay and an oxidative damage model in alpha mouse liver 12 (AML-12) cells to protect them from oxidative damage (Figure 4C,D).⁷² In addition, MXenes can be used as nanozymes to treat oxidative stress-related illnesses because of their metallic conductivity, ease of synthesis, high stability, catalytic activity, and cost-effectiveness. Feng et al. fabricated 2D V₂C MXenes that mimic different natural enzymes, namely catalase (CAT), glutathione peroxidase (GPx), haloperoxidase, peroxidase (POD), superoxide dismutase (SOD), and thiol peroxidase.^{74–76} Wang et al. fabricated AuNPs-decorated MXene NSs for colorimetric detection of penicillin G (PenG) in such real matrices.⁷⁷ With an LOD of 7.51 nM, the assay showed maximum residue limits for raw milk, generating superoxide anions and thus playing a crucial role in PenG catalysis.

In addition to directly catalyzing intracellular species, the MXene surface's highly electroactive functionalities, along with

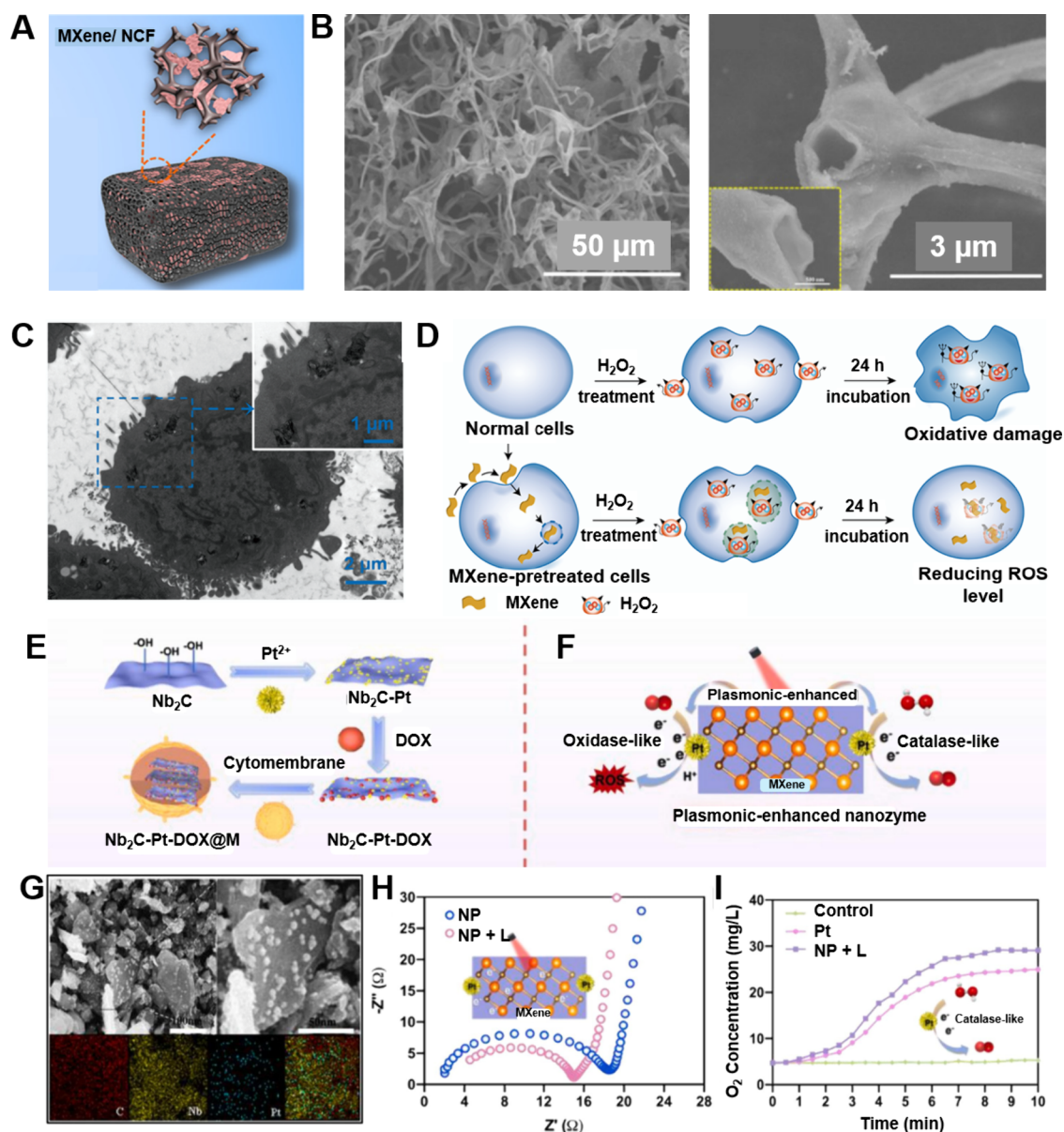


Figure 4. Bio-related catalytic and sensing functions of MXenes. (A) Schematic illustration of the preparation process for the MXene/NCF composite. (B) SEM morphologies of the MXene/NCF. The compressible MXene/N-doped carbon foam exhibits a unique neuron-like architecture. Reproduced with permission from ref 65 Copyright 2023, American Chemical Society. (C) TEM images of AML-12 cells treated with $50 \mu\text{g}\cdot\text{mL}^{-1}$ $\text{Ti}_3\text{C}_2\text{T}_x$. (D) Schematic illustration of the intracellular protective effect of MXenes. Reproduced with permission from ref 71 Copyright 2022, Springer Publishers. (E) Schematic illustration of the preparation of the biomimetic plasmonic assembly NP@M. (F) Catalytic process of plasmonic-enhanced nanozyme. (G) SEM images and EDS element mapping of Nb_2C -Pt. (H) EIS Nyquist plots of NP with or without 1064 nm laser irradiation ($0.5 \text{ W}/\text{cm}^2$). (I) Quantitative dissolved oxygen generation under saline, Pt, NP + L after the reaction with $0.1 \text{ mmol L}^{-1} \text{H}_2\text{O}_2$. Reproduced with permission from ref 72 Copyright 2021, Elsevier.

its metallic conductivity and biocompatibility, enable it to immobilize supramolecular biological components, including tyrosinase (Tyr),⁷⁷ lipase,⁷⁸ glucose oxidase,⁷⁹ and laccase.⁴⁸ These components enable the development of various biosensing monitoring systems.⁸⁰ Several other precursors have been used to improve the performance of immobilized enzymes on MXenes, such as NDs (Au,⁸¹ Pt,⁷⁵ CuS,⁷⁴ and CeO_2 ,⁸² MOFs⁴⁷/COFs,⁷⁸ and polymers (cellulose,⁸³ chitosan⁷⁹ and biomembranes⁷² towards gas and cancer sensing. Yu et al. fabricated a DNA electrochemical biosensor by combining a cleavage-ligation logic transcription circuit-activated DNAzyme

and MXene-Au dots to detect flap endonuclease 1 (FEN1) activity.⁸¹ Ao et al. designed the composites based on encapsulating Candida albicans lipase B (CalB) in a cyclodextrin-MOFs loaded with $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes through *in situ* growth.⁴⁷ These composites not only protected the highly fragile enzyme but also enhanced its catalytic ability. Wu et al. designed a Ti_3C_2 matrix to immobilize the Tyr enzyme, thereby fabricating a mediator-free biosensor for phenol detection.⁷⁷ Mechanistically, the phenol could be oxidized in an oxygen-containing environment to an *o*-quinone, which could then be electrochemically reduced at the electrode surface to a

Table 1. A Summary of Diverse Precisely MXene-Derived Nanoarchitected Composites for Various Catalytic Applications

applications	guest & host	type of MXenes	size	outcome	ref.
Biocatalysis	CuS nanospheres on MXenes	Ti ₃ C ₂	173.7 nm	Achieved sensitive MRSA detection (LOD: 6–7 CFU/mL) with concurrent bacterial inactivation.	74
	Pt single atom on MXenes	Ti ₃ C ₂		Enabled efficient bacterial killing and biofilm removal via NIR-enhanced catalysis (76.4% photothermal efficiency).	75
	Gold nanoparticles on MXenes	Ti ₃ C ₂ T _x		Enabled sensitive PenG detection via catalase-like activity (LOD: 7.51 nM), below the US-FDA/EU MRLs.	76
	CeO ₂ nanoclusters on MXenes	Ti ₃ C ₂		Demonstrated catalase-like multianalyte sensing of H ₂ O ₂ and enzyme-coupled metabolites, with detection down to 0.49 μM.	82
	Pt nanozymes on MXenes	Nb ₂ C	<10 nm	Promoted NIR-II-triggered O ₂ /ROS generation and enhanced cancer-cell internalization.	72
	Gold NDs on MXenes and load a substantial amount of capture DNA	Ti ₃ C ₂		Demonstrated sensitive and specific FEN1 activity detection with good reproducibility.	81
Electrocatalysis	Co ₃ O ₄ nanoparticles on MXenes	Ti ₃ C ₂	~50 nm	Achieved efficient OER activity with a low overpotential of 300 mV at 10 mA·cm ⁻² and improved kinetics over bulk Co ₃ O ₄ .	84
	NiFe ₂ O ₄ nanoparticles decorated on MXenes	Ti ₃ C ₂		Provided efficient bifunctional electrocatalysis for both OER and HER using NiFe ₂ O ₄ /Ti ₃ C ₂ composites.	85
	Ni-doped MoSe ₂ nanoflowers on MXenes	Ti ₂ NT _x	100~200 nm	Enhanced alkaline overall water-splitting performance through improved HER and OER activity in Ni–MoSe ₂ /Ti ₂ NT _x heterostructures.	86
	CoNi LDH coated on MXenes	Ti ₃ C ₂ T _x		Demonstrated strong alkaline OER activity with a low overpotential of 257.4 mV at 100 mA/cm ² .	87
	Co single atoms on MXenes	Mo ₂ C		Achieved favorable OER kinetics through optimized OH adsorption, with a low overpotential of 270 mV at 10 mA/cm ² .	88
	Ce-MOF on MXenes	Ti ₃ C ₂		Delivered durable multifunctional HER/OER and supercapacitor performance, with retention of up to 99.7%.	89
Heterogeneous catalysis	Carbon nanotube between MXenes	Ti ₃ C ₂ T _x		Combined high-capacity LIB storage (491 mA h g ⁻¹) with efficient HER activity (93 mV at 10 mA cm ⁻²).	90
	Cu ₃ cluster doped on MXenes	Mo ₂ CO ₂		Enhanced CO oxidation through Cu ₃ -cluster-mediated electron transfer regulation on Mo ₂ CO ₂ .	91
	Pt-doped MXenes	Ti ₃ C ₂		Maintained >90% benzene conversion under humid conditions with stable performance over seven cycles.	92
	Gold nanoparticles on PNIPAM/MXenes	Ti ₃ C ₂	17.4 nm	Showed switchable catalytic activity for 4-NP reduction through thermoresponsive MXene nanocomposite design.	93
	Pt atoms anchored on MXenes.	Ti ₃ C ₂ T _y		Facilitated selective CO ₂ fixation to amides, with a markedly higher TON than Pt nanoparticles.	94
	Pd/Cu nanoparticles on MXenes	Ti ₃ C ₂	5–10 nm	Enabled ligand-free Suzuki–Miyaura coupling with high yields and stable catalytic performance over at least 10 cycles.	95
Photocatalysis	Pt nanoparticles on MXenes	Nb ₂ C	~2.6 nm	Regulated WGS kinetics through reduction-induced strong metal–support interactions that modulate CO adsorption and H ₂ O activation.	96
	Pt quantum dots and TiO ₂ nanowires on MXenes	Ti ₃ C ₂ T _x	72.095 nm (Pore size)	Boosted artificial-solar-light CO ₂ reduction through Pt QD synergism, reaching 4.8-fold higher activity than pristine Ti ₃ C ₂ .	55
	Cu ₂ O/BiVO ₄ nanocomposites on MXenes	Ti ₃ C ₂		Achieved near-complete TC mineralization with simultaneous H ₂ evolution (4.70 mmol·g ⁻¹ ·h ⁻¹) and CO ₂ conversion to CO/CH ₄ under visible light.	97
	Bi-MOF deposited on MXenes	Ti ₃ C ₂	30~100 nm	Delivered additive-free NH ₃ production in pure water via the CAU-17/MXene Schottky heterojunction (56.34 μmol·g ⁻¹ ·h ⁻¹).	98
	CdS nanorod on MXenes	Ti ₃ C ₂	100 nm	Produced a 7-fold enhancement in H ₂ generation through intimate interfacial contact and accelerated charge transport.	99
	Bi ₂ O ₂ SiO ₃ nanosheet on MXenes	Ti ₃ C ₂		Enhanced solar-driven CO ₂ reduction with a CO yield of 17.8 μmol·g ⁻¹ ·h ⁻¹ and ~90% selectivity over CH ₃ OH.	100
	g-C ₃ N ₄ nanosheet on MXenes	V ₂ C		Enhanced photocatalytic CH ₄ production to 205 μmol·g ⁻¹ , reaching 6.7-fold higher activity than pristine g-C ₃ N ₄ .	101
	Ag ₃ PO ₄ nanoparticles on MXenes	Ti ₃ C ₂	100–200 nm	Achieved broad-spectrum visible-light degradation of multiple organic pollutants using the self-assembled Ag ₃ PO ₄ /Ti ₃ C ₂ Schottky catalyst.	102
	AgInS ₂ nanoparticles on MXenes	Ti ₃ C ₂	~22 nm	Achieved efficient visible-light N ₂ fixation, with 30 wt% AgInS ₂ reaching 38.8 μmol/(g·h).	103
	MIL-100(Fe) nanoparticles on MXenes	Ti ₃ C ₂		Improved photocatalytic NO oxidation to 57.92%, achieving 4-fold and 3-fold higher efficiency than Ti ₃ C ₂ and MIL-100(Fe), respectively.	104

polyhydric phenol, amplifying the phenol signal. The varied electrochemical measurements revealed the electrochemical performance of these MXene-based composites, with a wide linear range from 0.05 to 15.5 μmol L⁻¹. The chitosan-encapsulated Tyr-immobilized Ti₃C₂ matrix showed unique performance with rapid response, high sensitivity (414.4 mA M⁻¹), and a low detection limit (12 nmol L⁻¹). The proposed enzyme-based biosensor design is evidenced by robust electrochemical biosensing, with excellent repeatability and reproducibility, long-term stability, and high recovery for sample detection in water.

Although these composites have been used for biosensing applications, biocatalysis-based nanomedicines could be used more broadly for therapeutic purposes to improve catalytic activity. Hao et al. generated a photoinduced plasmonic assembly integrating Nb₂C plasmon (MXenes) and Pt nanozymes (NPD@M), encapsulated with tumor cell membranes for DOX delivery (Figure 4E–I).⁷² The designed composites, featuring exceptional CAT-like and oxidase-like activities of Pt nanozymes, alleviated hypoxia by producing O₂ and ROS, thereby improving PTT-assisted cancer therapy in the second near-infrared (NIR-II) biological window. The plasmonic

assembly alleviated cancer growth both *in vitro* and *in vivo*. In addition, MXene-loaded single-atom catalysts (Pt-Ti₃C₂) hybridized at their Ti vacancies were designed for anti-infective therapy.⁷⁵ These composites with POD-like activity effectively ablated bacteria and eradicated biofilm through locally catalyzing hydrogen peroxide to generate deadly hydroxyl radicals. These MXenes encapsulated with single-atom catalysts demonstrated photothermally induced biocatalysis-based therapy against bacteria and cancer, towards the development of biocatalytic nanomedicines.

Three design principles dominate contemporary MXene electrocatalysis research: 1) surface termination engineering tunes adsorption energetics; 2) Defect and compositional engineering strategies create discrete active centers; 3) Heterostructuring and hybridization approaches address practical performance limitations.¹⁰⁵ While the intrinsic electrical conductivity of MXenes facilitates fast electron transfer, their long-term stability and surface reconstruction behavior under operating potentials remain mechanistic open challenges. Understanding whether MXenes act as true catalytic phases or as dynamic precursors forming oxide/oxyhydroxide intermediates is central to mechanistic attribution.¹⁰⁶ Water splitting proceeds through two half-reactions with distinct mechanistic challenges: the HER ($2\text{H}^+ + 2\text{e}^- \rightarrow \text{H}_2$ in acid, or $2\text{H}_2\text{O} + 2\text{e}^- \rightarrow \text{H}_2 + 2\text{OH}^-$ in base) at the cathode¹⁰⁷ and the OER ($4\text{OH}^- \rightarrow \text{O}_2 + 2\text{H}_2\text{O} + 4\text{e}^-$ or $2\text{H}_2\text{O} \rightarrow \text{O}_2 + 4\text{H}^+ + 4\text{e}^-$) at the anode.¹⁰⁸ Density functional theory (DFT) studies revealed that oxygen-terminated MXenes, such as Ti₂CO₂ and V₂CO₂, exhibit near-thermoneutral ΔGH values, whereas fluorine-terminated analogs bind hydrogen too weakly.¹⁰⁹ A growing body of *operando* evidence indicated that MXene surfaces could undergo structural and chemical reconstruction during prolonged HER operation, often forming thin oxide or oxyhydroxide layers towards catalytic applications. Nevertheless, the mechanistic challenge, therefore, lies in distinguishing the intrinsic activity of the pristine MXene from that of its electrochemically evolved derivative. Addressing this ambiguity requires combined theoretical and *operando* spectroscopic studies. Mechanistically, OER often proceeds via the adsorbate evolution mechanism (AEM), which involves the sequential formation and transformation of *OH, *O, and *OOH intermediates at the catalyst surface.¹¹⁰ Under anodic conditions, partial oxidation of MXene surfaces often leads to the formation of oxy-carbide or oxyhydroxide layers, which can participate in lattice oxygen-mediated (LOM) pathways. In such mechanisms, lattice oxygen atoms from the catalyst itself are directly involved in the O–O bond formation step, exchanging with adsorbed species to generate molecular oxygen.¹⁷ Despite these strengths, oxidative stability remains a key mechanistic challenge for many MXenes, particularly Mo- and V-based analogues, which tend to form oxide layers at high anodic potentials. These surface oxides can either suppress conductivity or, intriguingly, evolve into the true catalytic phase responsible for OER activity.

Nevertheless, pure MXenes typically exhibit weak oxygen binding because their metal–carbon/nitrogen frameworks are relatively inert and often terminated by electronically passivating groups such as –F. When terminations are replaced with –O or –OH, the local electronic structure around the transition-metal sites changes, enhancing interaction with oxygen intermediates and tuning the surface toward optimal adsorption energetics.¹¹¹ For example, studies on Ti₄N₃ MXene showed that OH-termination significantly enhanced

electrocatalytic activity by stabilizing *OOH intermediates and lowering the overpotential in alkaline media. In addition, introducing metal dopants (Fe, Co, or Ni) or non-metal dopants (N, P, or S) enabled the local modulation of the electronic density of states, thereby tailoring binding energies and enhancing catalytic turnover.¹¹² Interfacial engineering *via* graphene/MXene heterostructures further optimized hydrogen adsorption energetics, with reaction free-energy profiles and atomic-level transition states confirming synergistic activity enhancement through N-doped graphene coupling. *Operando* spectroscopic studies indicated that such transformations might be partially reversible, suggesting that controlled oxidation could be harnessed as a principle rather than viewed solely as a degradation pathway. Collectively, these mechanistic insights underscore how MXenes, through their tunable surface chemistry, high conductivity, and adaptive reconstruction behavior, can serve as efficient bifunctional materials for both HER and OER. Their ability to balance structural stability with dynamic surface activation represents a key advantage for designing durable, high-performance water-splitting electrocatalysts.¹¹³ Electronic coupling between graphene and MXene surfaces, as shown by shifts in the C p_z-band center and the correlation between work function and *OH binding energies, indicates that interfacial orbital hybridization governs adsorption energetics and electron-transfer efficiency.

In hybrid architectures, MXenes act as electron highways, strongly coupling with conductive or catalytically active phases such as nitrogen-doped carbon, transition-metal oxides, or metallic nanoparticles (Table 1).¹¹⁴ The interfacial charge-transfer behavior of Pt/MXene hybrids with different terminations is depicted.^{107,115} Such interfacial coupling enables charge redistribution across the interface, promoting polarization of oxygen intermediates and accelerating reaction kinetics.¹¹⁶ For instance, coupling MXenes with N-doped graphene enhances p_z orbital overlap, improving the rate of electron transfer and lowering activation barriers for O–O bond cleavage.^{111,117} Moreover, defects and variable surface terminations on MXenes create efficient tunneling pathways that facilitate electron flow from the host lattice to adsorbed *O₂ or *OOH species. These conductive and interfacial advantages collectively account for the superior ORR kinetics often observed in MXene-based composite catalysts.¹¹⁸ Long-term durability studies reveal morphological changes, partial oxidation, and metal leaching, suggesting that the distribution and identity of active sites evolve continuously during operation. The projected density of states (PDOS) analysis and a schematic of orbital hybridization further support the idea that σ/σ^* coupling between MXene and graphene orbitals facilitates delocalized charge transport and balanced intermediate binding.¹¹⁷ Understanding and controlling these dynamic transformations remains a key frontier for mechanistic elucidation and long-term catalyst stability. Despite the apparent diversity in their reaction coordinates, these transformations share a common mechanistic foundation rooted in the interplay of intermediate adsorption energetics, charge-transfer efficiency, surface reconstruction dynamics, and the delicate balance between catalytic stability and reactivity. Moreover, several critical mechanistic challenges persist. Importantly, identifying true active sites and distinguishing between pristine MXenes, reconstructed oxides, and dopant-derived phases under operating bias remains a non-trivial task. Together, MXene-based materials provide an adaptable mechanistic platform for modulating HER & OER

energetics, electron transfer, and reaction selectivity while also revealing the complexity of surface dynamics under realistic electrochemical conditions.

MXenes can serve as heterogeneous catalysts for some organic reactions because of their high electrical conductivity, large surface area, and tunable surface chemistry. The redox-active sites involve the transition-metal centers, differentiating them from traditional metal-free organocatalysts. Specifically, these MXenes primarily act as catalyst supports for various organic transformations. Nevertheless, pristine MXenes are prone to oxidation or delamination during catalysis, limiting their applicability in heterogeneous catalysis. Auxiliary components (Pt species, Au dots, MoS₂ NSs, and polymers) immobilized on MXenes improve structural stability and expose various terminal active sites, thereby maintaining long-term catalytic activity (Table 1).⁹⁶ Although their roles have been explored for various catalytic applications (photo-, electro-, and thermal-based catalysis), MXene-based composites in organic reactions remain limited. In this section, we emphasize the roles of various MXene-based composites in organic transformations, including oxidation, reduction, ring opening, and C–H activation reactions (Figure 5).

Several studies have explored the utilization of MXenes (vanadium carbide, V₂C) to demonstrate their catalytic activity. Dhakshinamoorthy et al. demonstrated the aerobic oxidation of indane to a mixture of indanol/indanone using molecular oxygen.¹¹⁹ In addition, they demonstrated the roles of surface hydroxyl groups, including surface oxidation with ammonium persulfate to convert some surface groups into oxo groups and surface dehydroxylation *via* thermal treatment under a diluted hydrogen flow. However, MXenes are often prone to oxidative degradation, leading to oxide formation and composites (TiO₂/Ti₃C₂T_x) and a loss of catalytic activity. Encapsulating MXenes with protective agents (carbonaceous materials, bentonite, and tannic acid) can regulate their intrinsic oxidation and enhance performance in certain environments.¹²⁰ Notably, researchers have explored the oxidation process using these MXene-based

composites for removing toxic pollutants, such as CO oxidation. Interestingly, Cheng et al. presented Cu₃-cluster-decorated pristine and defective Mo₂CO₂ monolayers for CO oxidation.⁹¹ Comparatively, Cu₃/d-Mo₂CO₂ showed superior catalytic performance, with exceptional stability and reactivity. Wang et al. fabricated Pt@Ti₃C₂ composites for the low-temperature oxidative removal of benzene under varied reaction conditions, including reaction temperature, Pt amount, and benzene concentration.⁹² The catalytic oxidation improved with increasing amounts of the guest Pt species on MXenes.

MXenes decorated with Au dots exhibited exceptional catalytic activity as reducing agents, owing to their active catalytic sites. The polymer coating effectively reduced MXene stacking and protected structural stability. In one case, an innovative core-shell structured MXene-COOH@(PEI/PAA)_n@AuNPs was prepared using layer-by-layer assembly of polymers (PEI and polyacrylic acid) over MXenes and subsequent decoration of Au NPs.¹²¹ These composites, with better thermal stability, exhibited exceptional catalytic reduction of nitro compounds (nitrophenol) with NaBH₄. This approach achieved repeatability above 90% even after 8 successive catalytic cycles, demonstrating recyclability and suitable stability. Similarly, poly(*N*-isopropylacrylamide) chains were grafted on the surface of Au NPs-decorated MXenes with a self-reduction property for the reduction of nitrophenol at room temperature.⁹³ Interestingly, the reaction could be terminated due to the polymer's temperature sensitivity at elevated temperatures (40 °C). This smart ON/OFF regulation, with tunable catalytic activity, could be promising for industrial use.

The designed composites efficiently reduce hazardous chemical intermediates, enhancing their potential in catalysis and wastewater treatment. Chen et al. proposed single-atom catalysts via a simultaneous self-reduction stabilization process, in which Pt₁/Ti_{3-x}C₂T_y provided a green route for utilizing the greenhouse gas CO₂ through the formylation of amines.⁹⁴ Pt-doped MXenes significantly reduced adsorption energy, thereby boosting their catalytic reduction performance. A ring-opening

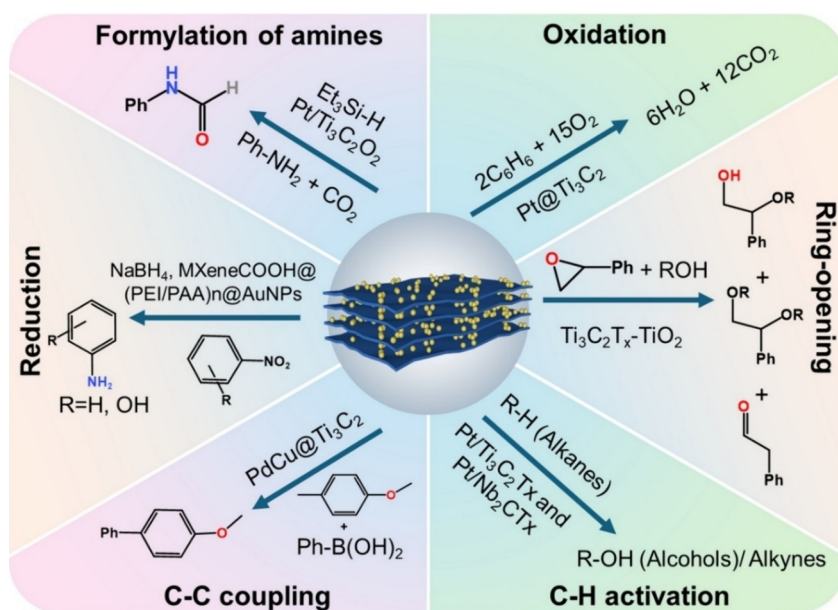


Figure 5. Catalytic performance of MXenes and their composites in heterogeneous catalysis, involving oxidation, reduction, formylation, C–C coupling, C–H activation, and epoxide ring-opening reactions.

reaction opens cyclic monomers into reactive functional groups, leading to long polymer chains through chain-growth polymerization (e.g., caprolactone to polycaprolactone). Considering the surface functional groups (O, OH, and/or F atoms), 2D MXenes can be employed as excellent acid catalysts for ring-opening reactions. Slot et al. demonstrated enhanced selectivity for catalytic epoxide ring-opening with surface-functionalized MXenes ($\text{Ti}_3\text{C}_2\text{T}_x$).¹²² The oxidized $\text{Ti}_3\text{C}_2\text{T}_x$ surfaces, upon conversion to TiO_2 , regulated reaction kinetics and selectivity for the epoxide ring-opening of styrene oxide (SO) and its isomerization in the liquid phase. Accordingly, controlling the type and number of acid sites on the MXene surface for SO ring-opening catalysis could help regulate selectivity and catalytic activity.

C–H bond activation is often used to prepare organometallic compounds, which bacteria employ to use natural resources efficiently. Typically, this attractive strategy enables the introduction of chemical functionalities. Towards fabricating exceptional catalysts and their supports using MXenes, Li and colleagues demonstrated metal-support interactions on Pt/ $\text{Ti}_3\text{C}_2\text{T}_x$ and Pt/ Nb_2CT_x catalysts for C–H activation.¹²³ The Pt/ $\text{Ti}_3\text{C}_2\text{T}_x$ showed a lower d-band center than Pt alone, which might have led to weaker adsorption of light hydrocarbon species. Accordingly, a lower olefin desorption barrier increases the contribution of C–C bond dissociation to high catalytic activity. Compared with Pt/ $\text{Ti}_3\text{C}_2\text{T}_x$, the Pt/ Nb_2CT_x catalyst showed slightly lower selectivity, possibly due to differences in IMC extent and electronic effects. Shen et al. fabricated a heterogeneous catalyst based on $\text{PdCu@Ti}_3\text{C}_2$ using a one-step reduction method. The researchers evaluated the composites for catalytic efficiency in the Suzuki–Miyaura cross-coupling reaction. Accordingly, $\text{PdCu@Ti}_3\text{C}_2$ showed exceptional catalytic activity, comparable to that of homogeneous Pd-based catalysts such as $\text{Pd}(\text{PPh}_3)_4$.⁹⁵ Interestingly, the authors indicated that the fabricated heterogeneous MXene-based catalyst could be used at least 10 times for the Suzuki–Miyaura coupling reaction with exceptional yields, thereby promoting green chemistry.

Photocatalysis is an advanced oxidation process that utilizes light energy to drive redox reactions at the surface of a semiconductor for solar energy conversion, hydrogen generation, CO_2 reduction, and pollutant degradation.¹²⁴ Photocatalytic efficiency depends on the material's ability to absorb light, generate charge carriers (electrons and holes), and transfer them effectively to reactive sites. However, conventional semiconductor photocatalysts, such as TiO_2 , CdS, ZnO, and $g\text{-C}_3\text{N}_4$, face intrinsic challenges, including rapid electron–hole recombination, limited visible-light absorption, and poor stability. In this context, MXenes and their composites offer distinct advantages: excellent electrical conductivity facilitates charge-carrier transport; surface functionalities provide active sites for adsorption and redox reactions; and a layered structure allows intimate interfacial contact with other semiconductors to form efficient heterojunctions.²⁹ Accordingly, photocatalysis can occur through multiple mechanisms, including acting as electron mediators, supports, or co-catalysts. The metallic conductivity of MXenes enables them to act as electron sinks, facilitating the rapid transfer of photogenerated electrons from the semiconductor to the MXene surface. This process reduces electron–hole pair recombination, thereby increasing charge-carrier lifetime. The formation of Schottky junctions between MXenes and semiconductors, such as $\text{TiO}_2/\text{Ti}_3\text{C}_2\text{T}_x$ or $\text{CdS}/\text{Ti}_3\text{C}_2$, is key to this function. In these systems, the

MXene Fermi level lies below the semiconductor conduction band, allowing electrons to flow into the MXene while holes remain in the semiconductor. The directional charge separation significantly enhances photocatalytic efficiency.

In addition, MXenes serve as robust supports for semiconductor nanostructures due to their mechanical strength, large surface area, and abundant nucleation sites for nanoparticle growth, ensuring uniform dispersion and preventing aggregation. For instance, Ti_3C_2 -supported MoS_2 NSs showed improved HER activity because of their high surface exposure. Moreover, MXenes can limit photocatalyst particle size, creating quantum confinement effects that further enhance light absorption and catalytic activity. Another critical role of MXenes is enhanced reactant adsorption. The negatively charged surfaces effectively adsorb positively charged pollutants or reactive intermediates, while their interlayer spacing can store CO_2 molecules or H_2O for subsequent reactions. In addition, they modulate catalytic selectivity; for example, $-\text{O}$ -terminated Ti_3C_2 exhibits optimal Gibbs free energy for hydrogen adsorption ($\Delta G_{\text{H}} \approx 0$ eV), making it an excellent substitute for expensive platinum in photocatalytic hydrogen generation.¹²⁵ MXenes have been successfully integrated into various photocatalytic applications, including water splitting, CO_2 reduction, pollutant degradation, and nitrogen fixation. MXenes (Ti_2C , Ti_3C_2 , and Nb_2C) are widely used as co-catalysts with semiconductors such as CdS, TiO_2 , and $g\text{-C}_3\text{N}_4$. In $\text{Ti}_3\text{C}_2/\text{CdS}$ systems, the O-terminated Ti_3C_2 surface acts as an efficient electron acceptor, forming a Schottky barrier that facilitates charge separation and drives HER under visible light (Table 1). The 2D–2D $\text{Ti}_3\text{C}_2/g\text{-C}_3\text{N}_4$ heterojunction also exhibits superior H_2 generation efficiency, as intimate contact between the layers promotes fast charge transfer and inhibits recombination. The resultant Ti_3C_2 -transformed NDs as composites display even higher activity due to the increased number of surface-active sites and stronger interfacial coupling.¹²⁶ MXene-based photocatalysts have demonstrated remarkable capability for converting CO_2 into hydrocarbons or alcohols. The layered structure of MXenes provides abundant adsorption sites for CO_2 molecules, while their metallic nature facilitates multi-electron transfer reactions. $\text{Ti}_3\text{C}_2/\text{Bi}_2\text{WO}_6$ and Nb_2CT_x composites have demonstrated efficient conversion of CO_2 to CO and CH_4 under visible light. The synergistic effect between MXene's conductivity and the semiconductor's photoactivity enables effective utilization of solar energy for carbon-neutral fuel production.⁹⁷

MXene-based systems are also highly effective in degrading organic dyes and contaminants in water. The $\text{Ti}_3\text{C}_2/\text{CdS}$ and $\text{Ti}_3\text{C}_2/\text{TiO}_2$ composites have been extensively studied for breaking down pollutants such as rhodamine B, methylene blue, and nitroaniline. MXene not only enhances light absorption but also accelerates ROS ($\cdot\text{OH}$ and $\cdot\text{O}_2^-$) generation, which drives oxidative degradation. Additionally, MXene-derived TiO_2/C heterostructures demonstrate excellent stability, reusability, and resistance to photocorrosion, which are vital for long-term water purification systems.¹²⁷ Recent studies explored the potential of MXene-based photocatalysts for nitrogen fixation, converting atmospheric N_2 into NH_3 under mild conditions. Active metal sites (Nb, Ti, or V) and surface functionalities facilitate activation of $\text{N}=\text{N}$ bonds, while conductive layers shuttle electrons efficiently. Furthermore, MXenes have been applied to H_2O_2 generation, antibacterial treatment, and fuel desulfurization, expanding their utility

beyond conventional photocatalytic reactions.⁹⁸ Despite significant advances, several challenges remain in fully exploiting MXenes in photocatalysis, including poor chemical stability, as they are prone to oxidation in air or aqueous environments, which alters their structure and degrades performance. Developing surface passivation strategies or heterostructures that stabilize MXenes under operational conditions is a priority. Another challenge is precisely controlling surface terminations ($-O$, $-F$, and $-OH$), which significantly influence electronic properties and catalytic activity.

In conclusion, this review discusses the synthesis of various MXenes and their composites for diverse catalytic applications. In this article, we discussed the roles of these designed MXene-based composites in diverse catalytic applications. Despite significant advances, several challenges remain to fully exploit MXenes and their composites in catalysis, including reproducible synthesis, storage stability, and broader applicability (Figure 6). Future research should focus on rationally designing heterostructures with controlled orientation, tunable interlayer spacing, and tailored surface chemistry. Defect engineering, doping, and surface modification can further enhance charge separation and catalytic selectivity. Accordingly, advanced synthesis techniques such as plasma treatment, atomic layer deposition, and molecular intercalation can engineer desired surface functionalities, thereby enhancing stability and improving performance.

Furthermore, scalability and reproducibility remain key obstacles. Most MXene-based catalysts are produced using small-scale laboratory methods that involve HF-based etching, raising environmental and safety concerns. Exploring green synthesis routes, such as molten-salt etching or electrochemical exfoliation, could facilitate large-scale, environmentally friendly production. Integrating heterostructures into scalable architectures, such as membranes and electrodes, will enable their application in real-world energy and environmental systems. Translating these relationships into predictive design principles requires a multi-scale understanding, from atomic-scale interfacial bonding to macro-scale mass transport. Recently, *in situ* and *operando* characterization techniques have begun to map these connections directly, showing that a 3D macrostructure's pore-size distribution dictates reactant concentration gradients at the active site. The holistic view, linking atomic architecture to reactor-level performance, is crucial for transitioning from serendipitous material discovery to the rational engineering of MXene catalysts tailored for specific chemical environments and industrial process conditions.

The chemical instability of MXenes remains a major obstacle, as they tend to oxidize in air or aqueous environments, altering their structure and degrading performance. Developing surface passivation strategies or heterostructures that stabilize MXenes under operational conditions is thus a priority. Another

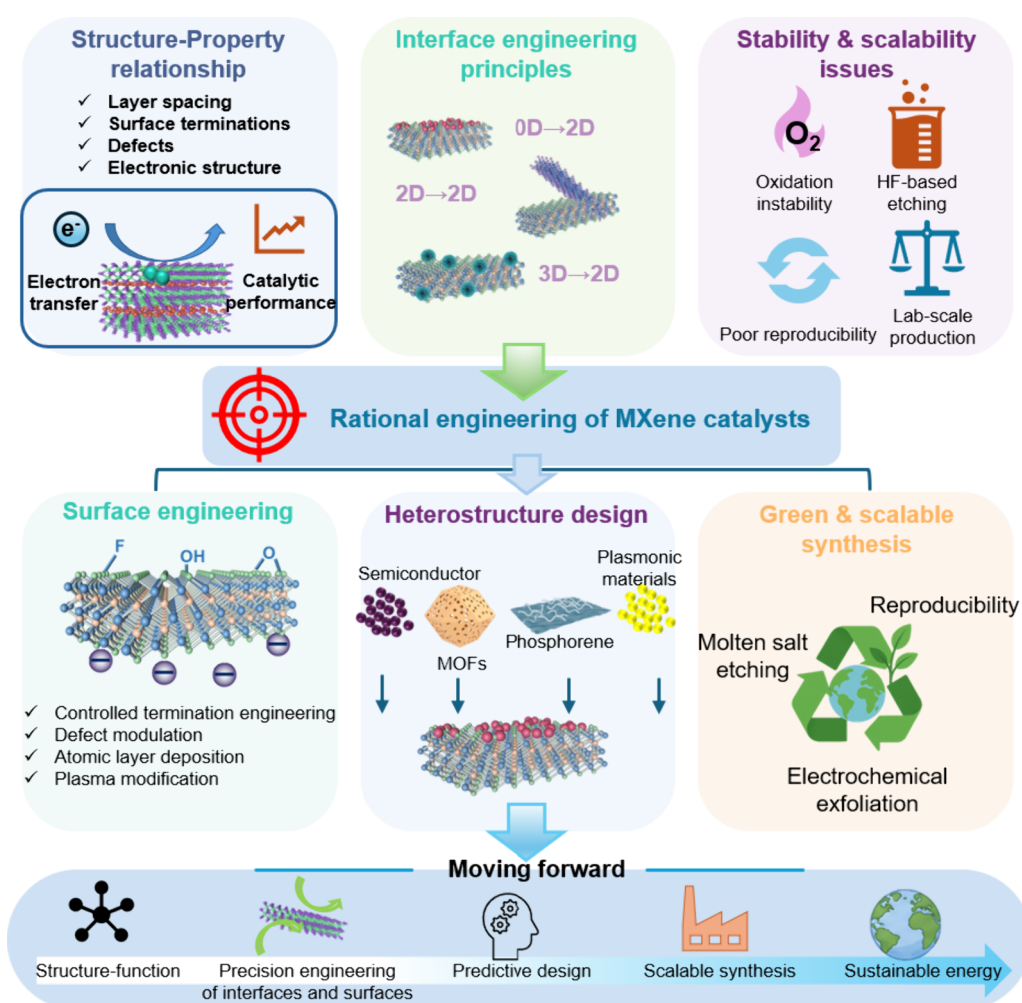


Figure 6. Schematic illustrating the outlook for the rational design of MXene composite nanoarchitectonics toward advanced catalytic applications.

challenge is precisely controlling surface terminations, as different terminations ($-O$, $-F$, and $-OH$) significantly influence electronic properties and catalytic activity. The future of MXene catalysis lies in rationally designing heterostructures. By coupling MXenes with narrow-bandgap semiconductors, plasmonic materials, or NDs and by exploring heterostructures based on novel 2D materials such as phosphorene, transition-metal carbides, and metal–organic frameworks, it is possible to extend light absorption into the visible or even the infrared region. Z-scheme and S-scheme heterojunctions fabricated with MXenes as conductive bridges maintain high redox activity while enhancing charge separation. Additionally, theoretical simulations based on DFT can guide the design of diverse MXene compositions and surface terminations tailored to specific catalytic reactions.¹²⁸

Coupling mechanisms provide a robust foundation for designing next-generation catalytic, electronic, and environmental technologies. Combining diverse 2D materials into coherent hybrid systems enables multifunctional devices that address global challenges in energy sustainability and environmental purification. As synthesis techniques mature and understanding of interfacial charge dynamics deepens, implementing these heterostructures in large-scale systems will become increasingly feasible. The field continues to expand, driven by interdisciplinary efforts that merge materials science, chemistry, and physics to unlock the full potential of engineering heterostructures. Ongoing exploration of 0D–2D, 2D–2D, and 3D–2D architectures not only enriches fundamental understanding of nanoscale interfaces but also paves the way for sustainable technologies that can reshape the future of energy and environmental innovation. Continued exploration of surface engineering, defect tuning, and heterostructure optimization will unlock further improvements in activity, selectivity, and durability. As synthesis methods become safer and more scalable, MXene-based materials are poised to play a crucial role in the global shift toward renewable energy and environmental sustainability.

■ ASSOCIATED CONTENT

Data availability Statement

No datasets were generated or analyzed, as this is a review manuscript.

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Notes

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REFERENCES

- (1) Astruc, D. Introduction: Nanoparticles in Catalysis. *Chem. Rev.* **2020**, *120*, 461–463.
- (2) Kankala, R. K.; Wang, S. B.; Chen, A. Z. Nanoarchitecting Hierarchical Mesoporous Siliceous Frameworks: A New Way Forward. *iScience* **2020**, *23*, 101687.
- (3) Joo, S. H.; Park, J. Y.; Tsung, C.-K.; Yamada, Y.; Yang, P.; Somorjai, G. A. Thermally stable Pt/mesoporous silica core-shell nanocatalysts for high-temperature reactions. *Nat. Mater.* **2009**, *8*, 126–131.
- (4) Huczko, A. Template-based synthesis of nanomaterials. *Appl. Phys. A* **2000**, *70*, 365–376.
- (5) Duan, C.; Yu, M.; Xu, J.; Li, B.-Y.; Zhao, Y.; Kankala, R. K. Overcoming Cancer Multi-drug Resistance (MDR): Reasons, mechanisms, nanotherapeutic solutions, and challenges. *Biomed. Pharmacother.* **2023**, *162*, No. 114643.
- (6) Sun, T.; Zhang, Y. S.; Pang, B.; Hyun, D. C.; Yang, M.; Xia, Y. Engineered nanoparticles for drug delivery in cancer therapy. *Angew. Chem., Int. Ed.* **2014**, *53*, 12320–12364.
- (7) Kankala, R. K.; Han, Y.-H.; Xia, H.-Y.; Wang, S.-B.; Chen, A.-Z. Nanoarchitected prototypes of mesoporous silica nanoparticles for innovative biomedical applications. *J. Nanobiotechnol.* **2022**, *20*, 126.
- (8) Duan, C.; Yu, M.; Zhao, Y.; Chen, X.; Kankala, R. K. Ternary Cu₂MX₄ (CMX)-based nanoarchitectonics: Chemistry, synthesis, and biomedical applications. *Coord. Chem. Rev.* **2024**, *518*, No. 216052.
- (9) Liong, M.; Lu, J.; Kovochich, M.; Xia, T.; Ruehm, S. G.; Nel, A. E.; Tamanoi, F.; Zink, J. I. Multifunctional Inorganic Nanoparticles for Imaging, Targeting, and Drug Delivery. *ACS Nano* **2008**, *2*, 889–896.
- (10) Kuthati, Y.; Kankala, R. K.; Lee, C.-H. Layered double hydroxide nanoparticles for biomedical applications: Current status and recent prospects. *Appl. Clay Sci.* **2015**, *112*, 100–116.
- (11) Gogotsi, Y.; Anasori, B. The Rise of MXenes. *ACS Nano* **2019**, *13*, 8491–8494.
- (12) Zhao, Y.; Wang, S.; Chen, A.; Kankala, R. K. Nanoarchitected assembly and surface of two-dimensional (2D) transition metal dichalcogenides (TMDCs) for cancer therapy. *Coord. Chem. Rev.* **2022**, *472*, No. 214765.
- (13) Li, W.; Qian, X.; Li, J. Phase transitions in 2D materials. *Nat. Rev. Mater.* **2021**, *6*, 829–846.
- (14) Ye, Y.-T.; Xiao, X.; Xia, H.-Y.; Li, J.; Gong, Z.-Z.; Chen, A.-Z.; Wang, S.-B.; Kankala, R. K. Photo-controlled spatiotemporal sequential release of MXenes/NO gas from bilayer (clean-cure) hydrogel promotes healing of MRSA biofilm-infected diabetic ulcer wounds. *J. Controlled Release* **2026**, *391*, No. 114611.
- (15) Alagarsamy, K. N.; Saleth, L. R.; Sekaran, S.; Fusco, L.; Delogu, L. G.; Pogorielov, M.; Yilmazer, A.; Dhinra, S. MXenes as emerging materials to repair electroactive tissues and organs. *Bioact. Mater.* **2025**, *48*, 583–608.
- (16) Hamzehlou, A.; Soroush, M. MXene-based catalysts: A review. *Mater. Today Catal.* **2024**, *5*, No. 100054.
- (17) Wu, X.; Wang, Y.; Wu, Z. S. Recent advancement and key opportunities of MXenes for electrocatalysis. *iScience* **2024**, *27*, No. 108906.
- (18) Verger, L.; Natu, V.; Carey, M.; Barsoum, M. W. MXenes: An Introduction of Their Synthesis, Select Properties, and Applications. *Trends Chem.* **2019**, *1*, 656–669.
- (19) Jawad, N. H.; Darwesh, T. M.; Abbas, A. F.; Yahya, A. A.; Kamel, A. H.; Rashid, K. T.; Abood, T. W.; Al-Juboori, R. A.; Meskher, H.; Al-Saadi, S.; et al. MXene Synthesis, Surface Functionalization, and Membrane Integration for Photocatalytic Removal of Heavy Metals from Wastewater: A Comprehensive Review. *Mater. Today Sustain.* **2025**, *32*, No. 101208.
- (20) Meng, Y.; Yue, F.; Zhang, S.; Zhang, L.; Li, C.; Shi, M.; Ma, Y.; Berrettoni, M.; Zhang, X.; Zhang, H. Zr-MOF/MXene composite for enhanced photothermal catalytic CO₂ reduction in atmospheric and industrial flue gas streams. *Carbon Capture Sci. Technol.* **2024**, *13*, No. 100274.
- (21) Rana, I.; Malakar, V. K.; Ranjan, K. R.; Verma, C.; AlFantazi, A.; Singh, P.; Kumari, K. MXenes and their composites for high-performance detection of pharmaceuticals and pesticides: A comprehensive review. *Composites, Part B* **2025**, *302*, No. 112521.
- (22) Ariga, K. Nanoarchitectonics: the method for everything in materials science. *Bull. Chem. Soc. Jpn.* **2024**, *97*, No. uoad001.
- (23) Ariga, K.; Yamauchi, Y. Nanoarchitectonics from Atom to Life. *Chem. Asian J.* **2020**, *15*, 718–728.
- (24) Long, Y.; Tao, Y.; Shang, T. X.; Yang, H. T.; Sun, Z. J.; Chen, W.; Yang, Q. H. Roles of Metal Ions in MXene Synthesis, Processing and Applications: A Perspective. *Adv. Sci.* **2022**, *9*, No. 2200296.
- (25) Thangavelu, H. H. S.; Huang, C. J.; Chabanais, F.; Palisaitis, J.; Persson, P. A Review on MXene Terminations. *Adv. Funct. Mater.* **2026**, *36*, No. e15604.
- (26) Cao, W.; Nie, J. L.; Cao, Y.; Gao, C. J.; Wang, M. S.; Wang, W. W.; Lu, X. L.; Ma, X. H.; Zhong, P. A review of how to improve Ti₃C₂T_x MXene stability. *Chem. Eng. J.* **2024**, *496*, No. 154097.
- (27) Chen, C.; Wang, B. Y.; Xu, J. J.; Fei, L. Y.; Raza, S.; Li, B. S.; Zeng, Q. Q.; Shen, L. G.; Lin, H. J. Recent Advancement in Emerging MXene-Based Photocatalytic Membrane for Revolutionizing Wastewater Treatment. *Small* **2024**, *20*, No. 2311427.
- (28) Zhou, Y. X.; Zhang, Y. L.; Ruan, K. P.; Guo, H.; He, M. K.; Qiu, H.; Gu, J. W. MXene-based fibers: Preparation, applications, and prospects. *Sci. Bull.* **2024**, *69*, 2776–2792.
- (29) Ali, M. M.; Hossen, M. A.; Aziz, A. A. Recent advances in synthesis of emerging MXenes photocatalysts: A systematic review. *J. Environ. Chem. Eng.* **2025**, *13*, No. 116877.
- (30) Zhang, Y.; Dong, C.; Ye, Z.; Hou, Y.; Ye, S. Engineering space dimension and surface chemistry of MXene-based nanocomposite photocatalysts for sustainable environmental applications. *Chem. Commun.* **2025**, *61*, 7158–7177.
- (31) He, L.; Zhuang, H.; Fan, Q.; Yu, P.; Wang, S.; Pang, Y.; Chen, K.; Liang, K. Advances and challenges in MXene-based electrocatalysts: unlocking the potential for sustainable energy conversion. *Mater. Horiz.* **2024**, *11*, 4239–4255.
- (32) Shuai, T.-Y.; Zhan, Q.-N.; Xu, H.-M.; Huang, C.-J.; Zhang, Z.-J.; Li, G.-R. Recent advances in the synthesis and electrocatalytic application of MXene materials. *Chem. Commun.* **2023**, *59*, 3968–3999.
- (33) Dhamodharan, D.; Al-Harthi, M. A.; Ramya, B.; Bafaqeer, A.; Alam, F. MXenes: A promising material with multifunctional applications. *J. Environ. Chem. Eng.* **2024**, *12*, No. 112316.
- (34) Ajmal, Z.; Qadeer, A.; Singh, K.; Al Mahmud, A.; Lakhan, M. N.; Pradeep, H.; Hussain, B.; Ullah, A.; Khan, H. R.; Ibrahim, E. H.; et al. A comprehensive review on MXenes for various applications. *Appl. Energy* **2025**, *397*, No. 126136.
- (35) Rahman, S. M. M.; Oliullah, M. S.; Arup, M. R.; Hasan, Z.; Islam, M. A.; Mim, J. J.; Hossain, N. Prospects and challenges of MXenes - a review. *Inorg. Chem. Commun.* **2025**, *180*, No. 115078.
- (36) Elyasi, G. S.; Ardjmand, M.; Arjmand, O. MXenes, properties and synthesis routes: A review. *Inorg. Chem. Commun.* **2025**, *180*, No. 114948.
- (37) Chirica, I. M.; Mirea, A. G.; Neatu, S.; Florea, M.; Barsoum, M. W.; Neatu, F. Applications of MAX phases and MXenes as catalysts. *J. Mater. Chem. A* **2021**, *9*, 19589–19612.
- (38) Lu, H.; Li, J.; Zhang, R.; Nie, K.; Li, Q.; Chen, Y.; Pan, F. Advances and perspectives of two-dimensional materials MXenes: Efficient catalysts for magnesium hydride. *Renewable Sustainable Energy Rev.* **2025**, *217*, No. 115759.
- (39) An, Y.; Tian, Y.; Feng, J.; Qian, Y. MXenes for advanced separator in rechargeable batteries. *Mater. Today* **2022**, *57*, 146–179.
- (40) Alam, A.; Saeed, G.; Mahmoudi, H.; Shakyia, J.; Tadesse, B. All MXene in-situ interfaced 0D/2D hybrid nanomaterials: 3D DIW printed asymmetric supercapacitor using binary Cu-Ni-O-FPs/

MXene and a-Fe-O-FPs/MXene electrodes. *Results Eng.* **2025**, *28*, No. 107167.

(41) Mostafavi, E.; Iravani, S. MXene-Graphene Composites: A Perspective on Biomedical Potentials. *Nanomicro Lett.* **2022**, *14*, 130.

(42) Jaffri, J. A.; Ihsan, M.; Bashir, S.; Selvaraj, J.; Ramesh, S.; Vengadaesvaran, B.; Samad, N. A. A.; Thiyahuddin, I.; Husaini, T.; Srinivasan, G.; et al. Investigating synthesis techniques for single-metal and multi-metal MXenes: Assessing methods, benefits, challenges and applications in hydrogen production. *Sustain. Mater. Technol.* **2025**, *45*, No. e01502.

(43) Liu, K.; Wang, L.; Fu, T.; Zhang, H.; Lu, C.; Tong, Z.; Yang, Y.; Peng, Y. Oxygen-functionalized Ti_3C_2 MXene/exfoliated montmorillonite supported S-scheme $\text{BiOBr}/\text{Bi}_2\text{MoO}_6$ heterostructures for efficient photocatalytic quinolone antibiotics degradation. *Chem. Eng. J.* **2023**, *457*, No. 141271.

(44) Wei, S.; Fu, Y.; Liu, M.; Yue, H.; Park, S.; Lee, Y. H.; Li, H.; Yao, F. Dual-phase MoS_2 /MXene/CNT ternary nanohybrids for efficient electrocatalytic hydrogen evolution. *NPJ 2D Mater. Appl.* **2022**, *6*, No. 25.

(45) Liu, X.; Wu, K.; Tang, Y.; Qi, N.; Zhang, Y.; He, Y.; Fu, M.; Ao, Y. Ti_3C_2 MXene-derived TiO_2 @C attached on Bi_2WO_6 with oxygen vacancies to fabricate S-scheme heterojunction for photocatalytic antibiotics degradation and NO removal. *Chin. Chem. Lett.* **2025**, *36*, No. 110882.

(46) Su, T.; Peng, R.; Hood, Z. D.; Naguib, M.; Ivanov, I. N.; Keum, J. K.; Qin, Z.; Guo, Z.; Wu, Z. One-Step Synthesis of Nb_2O_5 /C/ Nb_2C (MXene) Composites and Their Use as Photocatalysts for Hydrogen Evolution. *ChemSusChem* **2018**, *11*, 688–699.

(47) Ao, Q.; Jiang, L.; Song, Y.; Tong, X.; Jiang, T.; Lv, X.; Tang, J. Base on photothermal molecular transfer for efficient biocatalysis via enzyme@cyclodextrin metal-organic frameworks loaded MXene. *Carbohydr. Polym.* **2024**, *343*, No. 122454.

(48) Malati, M. L.; Abrahams, A.; Chauke, V.; Dlamini, L. N. Rhus vernicifera laccase immobilization on Ti_2N MXene as a potential biocatalyst in environmental remediation. *Emergent Mater.* **2023**, *6*, 245–260.

(49) Rasheed, T. 3D MXenes as promising alternatives for potential electrocatalysis applications: opportunities and challenges. *J. Mater. Chem. C* **2022**, *10*, 9669–9690.

(50) Dey, A.; Varagnolo, S.; Power, N. P.; Vangapally, N.; Elias, Y.; Dampney, L.; Jaato, B. N.; Gopalan, S.; Golrokhi, Z.; Sonar, P.; et al. Doped MXenes—A new paradigm in 2D systems: Synthesis, properties and applications. *Prog. Mater. Sci.* **2023**, *139*, No. 101166.

(51) Jaiswal, D.; Sharma, C.; Roy, S.; Pandey, P. K.; Quiyoom, A.; Kumar, V.; Chebrolu, S.; Rakshit, P. K.; Singh, J. K.; Bera, J. K. $\text{Ti}_3\text{C}_2\text{T}_x$ -based Zr/MXene for CO_2 capture and conversion. *Chem. Commun.* **2025**, *61*, 17693–17696.

(52) You, X.; Yin, P.; Zhang, K.; Fu, H.; Song, F.; Yu, S.; Tang, Z.; Yang, C.; Wei, S.; Meng, Q.; et al. DFT Investigation on Transition-Metal Cr-, Mo-, and W-Doped MXene Nb_2CO_2 Nanosheets: Implications for High-Performance H_2 , CO, and H_2S Gas Sensors. *ACS Appl. Nano Mater.* **2025**, *8*, 13993–14005.

(53) Anand, R.; Nissimagoudar, A. S.; Umer, M.; Ha, M.; Zafari, M.; Umer, S.; Lee, G.; Kim, K. S. Late Transition Metal Doped MXenes Showing Superb Bifunctional Electrocatalytic Activities for Water Splitting via Distinctive Mechanistic Pathways. *Adv. Energy Mater.* **2021**, *11*, No. 2102388.

(54) Serafin, J.; Bujaldón, R.; Sreńscek-Nazzal, J.; Kalamaga, A.; Gomez, E.; Vendrell, X.; Serra, A. Transition metal-doped TiO_2 and CeO_2 photocatalysts modified with Ti_3C_2 MXene for PMS-driven advanced oxidation of pharmaceutical pollutants. *Chem. Eng. J.* **2025**, *524*, No. 169005.

(55) Charyulu Devarayapalli, D.; Prabhakar Vattikuti, S. V.; Kim, D. J.; Lim, Y.; Kim, B.; Kim, G.; Lee, D. S. Platinum quantum dots-decorated MXene-derived titanium dioxide nanowire/ Ti_3C_2 heterostructure for use in solar-driven gas-phase carbon dioxide reduction to yield value-added fuels. *J. Energy Chem.* **2023**, *82*, 627–637.

(56) Bai, J.; Chen, W.; Hao, L.; Shen, R.; Zhang, P.; Li, N.; Li, X. Assembling Ti_3C_2 MXene into ZnIn_2S_4 - NiSe_2 S-scheme

heterojunction with multiple charge transfer channels for accelerated photocatalytic H_2 generation. *Chem. Eng. J.* **2022**, *447*, No. 137488.

(57) Qin, Y.; Li, H.; Lu, J.; Feng, Y.; Meng, F.; Ma, C.; Yan, Y.; Meng, M. Synergy between van der Waals heterojunction and vacancy in ZnIn_2S_4 /g- C_3N_4 2D/2D photocatalysts for enhanced photocatalytic hydrogen evolution. *Appl. Catal., B* **2020**, *277*, No. 119254.

(58) Lim, K. R. G.; Handoko, A. D.; Nemani, S. K.; Wyatt, B.; Jiang, H. Y.; Tang, J.; Anasori, B.; Seh, Z. W. Rational Design of Two-Dimensional Transition Metal Carbide/Nitride (MXene) Hybrids and Nanocomposites for Catalytic Energy Storage and Conversion. *ACS Nano* **2020**, *14*, 10834–10864.

(59) Kumar, P.; Singh, S.; Hashmi, S. A. R.; Kim, K.-H. MXenes: Emerging 2D materials for hydrogen storage. *Nano Energy* **2021**, *85*, No. 105989.

(60) Xu, Q.; Zhang, L.; Cheng, B.; Fan, J.; Yu, J. S-Scheme Heterojunction Photocatalyst. *Chem* **2020**, *6*, 1543–1559.

(61) Guo, T.; Xu, X.; Liu, C.; Wang, Y.; Lei, Y.; Fang, B.; Shi, L.; Liu, H.; Hota, M. K.; Al-Jawhari, H. A.; et al. Large-Area Metal–Semiconductor Heterojunctions Realized via MXene-Induced Two-Dimensional Surface Polarization. *ACS Nano* **2023**, *17*, 8324–8332.

(62) Yadav, M.; Kumar, M.; Sharma, A. Review of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene Nanosheets and their Applications. *ACS Appl. Nano Mater.* **2024**, *7*, 9847–9867.

(63) Wei, Y.; Soomro, R. A.; Xie, X.; Xu, B. Design of efficient electrocatalysts for hydrogen evolution reaction based on 2D MXenes. *J. Energy Chem.* **2021**, *55*, 244–255.

(64) Saadh, M. J.; Hassan, W. H.; Nemah, A. K.; Khaleel Jameel, M.; Sharma, P.; Kumar, A.; Abul Hasan, M.; Islam, S.; Zainul, R. Removal of erythrosine B dye from wastewater using Ca_2C and Ti_2C MXenes: A theoretical study. *J. Mol. Liq.* **2024**, *411*, No. 125784.

(65) Sun, L.; Song, G.; Sun, Y.; Fu, Q.; Pan, C. MXene/N-Doped Carbon Foam with Three-Dimensional Hollow Neuron-like Architecture for Freestanding, Highly Compressible All Solid-State Supercapacitors. *ACS Appl. Mater. Interfaces* **2020**, *12*, 44777–44788.

(66) Li, K.; Liang, M.; Wang, H.; Wang, X.; Huang, Y.; Coelho, J.; Pinilla, S.; Zhang, Y.; Qi, F.; Nicolosi, V.; et al. 3D MXene Architectures for Efficient Energy Storage and Conversion. *Adv. Funct. Mater.* **2020**, *30*, No. 2000842.

(67) Chen, H.; Shao, Y.; Liu, Y.; Liu, Z.; Wang, C.; Liu, W.; Yu, F.; Wang, Y.; Yuan, D.; Jiang, H. Electro-trapping uranium with a cost-effective and scalable ice-templated MXene/VMT electrode. *Chem. Commun.* **2025**, *61*, 18898–18901.

(68) He, D.; Yang, X.; Huang, D.; Yue, G.; Yang, L.; Zhao, P. Palladium-MXenes aerogel decorated by alkyne functionalized polyvinyl alcohol (PVA) as a highly efficient catalyst for electrocatalytic hydrogen evolution. *Chem. Phys. Lett.* **2022**, *805*, No. 139942.

(69) Faraji, M.; Parsaee, F.; Kheirmand, M. Facile fabrication of N-doped graphene/ $\text{Ti}_3\text{C}_2\text{T}_x$ (MXene) aerogel with excellent electrocatalytic activity toward oxygen reduction reaction in fuel cells and metal-air batteries. *J. Solid State Chem.* **2021**, *303*, No. 122529.

(70) Yi, M.; Li, N.; Lu, B.; Li, L.; Zhu, Z.; Zhang, J. Single-atom Pt decorated in heteroatom (N, B, and F)-doped ReS_2 Grown on Mo_2CT_x for efficient pH-universal hydrogen evolution reaction and flexible Zn–air batteries. *Energy Storage Mater.* **2021**, *42*, 418–429.

(71) Liu, J.; Lu, W.; Lu, X.; Zhang, L.; Dong, H.; Li, Y. Versatile $\text{Ti}_3\text{C}_2\text{T}_x$ MXene for free-radical scavenging. *Nano Res.* **2022**, *15*, 2558–2566.

(72) Hao, Z.; Li, Y.; Liu, X.; Jiang, T.; He, Y.; Zhang, X.; Cong, C.; Wang, D.; Liu, Z.; Gao, D. Enhancing biocatalysis of a MXene-based biomimetic plasmonic assembly for targeted cancer treatments in NIR-II biowindow. *Chem. Eng. J.* **2021**, *425*, No. 130639.

(73) Feng, W.; Han, X.; Hu, H.; Chang, M.; Ding, L.; Xiang, H.; Chen, Y.; Li, Y. 2D vanadium carbide MXenezyme to alleviate ROS-mediated inflammatory and neurodegenerative diseases. *Nat. Commun.* **2021**, *12*, 2203.

(74) Su, T.; Zhang, Y.; Chang, Y.; Lin, X.; Dong, M.; Wu, S.; Wang, Z.; Duan, N. Nanozyme meets pathogen: A M-MXene@CuS platform for triple-mode detection and synergistic inactivation of MRSA. *Chem. Eng. J.* **2025**, *519*, No. 165639.

- (75) Li, Z.; Xu, D.; Deng, Z.; Yin, J.; Qian, Y.; Hou, J.; Ding, X.; Shen, J.; He, X. Single-Atom-Catalyzed MXene-Based nanoplatform with Photo-Enhanced Peroxidase-Like activity nanotherapeutics for *Staphylococcus aureus* infection. *Chem. Eng. J.* **2023**, 452, No. 139587.
- (76) Wang, W.; Gunasekaran, S. MXene/Gold nanoparticles heterostructure as catalase mimic for colorimetric detection of penicillin G. *Chem. Eng. J.* **2024**, 482, No. 148693.
- (77) Wu, L.; Lu, X.; Dhanjai, W.; Z.-S.; Dong, Y.; Wang, X.; Zheng, S.; Chen, J. 2D transition metal carbide MXene as a robust biosensing platform for enzyme immobilization and ultrasensitive detection of phenol. *Biosens. Bioelectron.* **2018**, 107, 69–75.
- (78) Ao, Q.; Jiang, L.; Song, Y.; Tong, X.; Jiang, T.; Tang, J. Hierarchical MXene/Enzyme@Covalent Organic Framework Composite by Template Method for Photothermal-Enhanced Lipase Catalysis. *Small* **2025**, 21, No. 2411962.
- (79) Tong, X.; Jiang, L.; Ao, Q.; Lv, X.; Song, Y.; Tang, J. Highly stable glucose oxidase polyananogel@MXene/chitosan electrochemical biosensor based on a multi-stable interface structure for glucose detection. *Biosens. Bioelectron.* **2024**, 248, No. 115942.
- (80) Irvani, S.; Varma, R. S. MXene-Based Composites as Nanozymes in Biomedicine: A Perspective. *Nanomicro Lett.* **2022**, 14, 213.
- (81) Yu, S.; Wang, C.; Gu, T.; Dang, Y.; Zhu, J.-J.; Ma, J.; Zhou, Y. An ultrasensitive electrochemical biosensor based on logic transcription circuit-activated DNzyme amplifier for flap endonuclease 1 activity detection. *Sens. Actuators, B* **2024**, 415, No. 135986.
- (82) Khan, R.; Andreescu, S. Catalytic MXCeO₂ for enzyme based electrochemical biosensors: Fabrication, characterization and application towards a wearable sweat biosensor. *Biosens. Bioelectron.* **2024**, 248, No. 115975.
- (83) He, C.-X.; Lu, Z.-Z.; Yao, X.-H.; Chen, T.; Zhao, W.-G.; Wang, J.; Zhang, D.-Y. Construction of a precise temperature-controlled continuous-flow catalytic reactor based on cellulose and MXene with directional thermal pathway heating and enzyme immobilization. *Chem. Eng. J.* **2025**, 504, No. 158971.
- (84) Lu, Y.; Fan, D.; Chen, Z.; Xiao, W.; Cao, C.; Yang, X. Anchoring Co₃O₄ nanoparticles on MXene for efficient electrocatalytic oxygen evolution. *Sci. Bull.* **2020**, 65, 460–466.
- (85) Shinde, P. V.; Mane, P.; Chakraborty, B.; Sekhar Rout, C. Spinell NiFe₂O₄ nanoparticles decorated 2D Ti₃C₂ MXene sheets for efficient water splitting: Experiments and theories. *J. Colloid Interface Sci.* **2021**, 602, 232–241.
- (86) Zong, H.; Yu, K.; Zhu, Z. Heterostructure nanohybrids of N-doped MoSe₂ coupled with Ti₂NT_x toward efficient overall water splitting. *Electrochim. Acta* **2020**, 353, No. 136598.
- (87) Hu, L.; Li, M.; Wei, X.; Wang, H.; Wu, Y.; Wen, J.; Gu, W.; Zhu, C. Modulating interfacial electronic structure of CoNi LDH nanosheets with Ti₃C₂T_x MXene for enhancing water oxidation catalysis. *Chem. Eng. J.* **2020**, 398, No. 125605.
- (88) Kou, Z.; Zang, W.; Pei, W.; Zheng, L.; Zhou, S.; Zhang, S.; Zhang, L.; Wang, J. A sacrificial Zn strategy enables anchoring of metal single atoms on the exposed surface of holey 2D molybdenum carbide nanosheets for efficient electrocatalysis. *J. Mater. Chem. A* **2020**, 8, 3071–3082.
- (89) Li, S.; Chai, H.; Zhang, L.; Xu, Y.; Jiao, Y.; Chen, J. Constructing oxygen vacancy-rich MXene @Ce-MOF composites for enhanced energy storage and conversion. *J. Colloid Interface Sci.* **2023**, 642, 235–245.
- (90) Wang, X.; Wang, S.; Qin, J.; Xie, X.; Yang, R.; Cao, M. Constructing Conductive Bridge Arrays between Ti₃C₂T_x MXene Nanosheets for High-Performance Lithium-Ion Batteries and Highly Efficient Hydrogen Evolution. *Inorg. Chem.* **2019**, 58, 16524–16536.
- (91) Cheng, C.; Zhang, X.; Yang, Z.; Zhou, Z. Cu₃-Cluster-Doped Monolayer Mo₂CO₂ (MXene) as an Electron Reservoir for Catalyzing a CO Oxidation Reaction. *ACS Appl. Mater. Interfaces* **2018**, 10, 32903–32912.
- (92) Wang, J.; Vikrant, K.; Younis, S. A.; Kim, K.-H.; Heynderickx, P. M. Low-temperature oxidative removal of benzene from the air using titanium carbide (MXene)-Supported platinum catalysts. *Chemosphere* **2024**, 350, No. 141114.
- (93) Chen, S.; Li, X.; Jiang, P.; Peng, W.; Tang, J.; Li, L.; Ye, L.; Pan, S.; Peng, C. Thermoresponsive MXene nanocomposite catalyst with high activity and thermosensitivity for controlled heterogeneous catalysis. *Mater. Today Chem.* **2022**, 26, No. 101005.
- (94) Zhao, D.; Chen, Z.; Yang, W.; Liu, S.; Zhang, X.; Yu, Y.; Cheong, W.-C.; Zheng, L.; Ren, F.; Ying, G.; et al. MXene (Ti₃C₂) Vacancy-Confining Single-Atom Catalyst for Efficient Functionalization of CO₂. *J. Am. Chem. Soc.* **2019**, 141, 4086–4093.
- (95) Zhu, D.; Zheng, K.; Qiao, J.; Xu, H.; Chen, C.; Zhang, P.; Shen, C. One-step synthesis of PdCu@Ti₃C₂ with high catalytic activity in the Suzuki–Miyaura coupling reaction. *Nanoscale Adv.* **2022**, 4, 3362–3369.
- (96) Li, Z.; Cui, Y.; Wu, Z.; Milligan, C.; Zhou, L.; Mitchell, G.; Xu, B.; Shi, E.; Miller, J. T.; Ribeiro, F. H.; et al. Reactive metal–support interactions at moderate temperature in two-dimensional niobium-carbide-supported platinum catalysts. *Nat. Catal.* **2018**, 1, 349–355.
- (97) Zhang, Y.; Ali, A. B. M.; Osman, H.; Samad, S.; Abdulrahman, A.; Zhang, K.; Mahariq, I.; Kutliev, U.; Abduvokhidov, A. Engineering a Multifunctional Cu₂O/BiVO₄@Ti₃C₂ MXene Z-Scheme heterojunction for photocatalytic environmental Detoxification, H₂ Generation, and CO₂ reduction to CO and CH₄: Experimental modeling and mechanistic insights. *Sep. Purif. Technol.* **2025**, 369, No. 133110.
- (98) Sun, A.; Sun, M.; Zhang, R.; Zhu, H.; Xing, Y. Surface and interface engineering of CAU-17/MXene Schottky heterojunction for efficient photocatalytic nitrogen fixation. *Sep. Purif. Technol.* **2025**, 362, No. 131939.
- (99) Xiao, R.; Zhao, C.; Zou, Z.; Chen, Z.; Tian, L.; Xu, H.; Tang, H.; Liu, Q.; Lin, Z.; Yang, X. In situ fabrication of 1D CdS nanorod/2D Ti₃C₂ MXene nanosheet Schottky heterojunction toward enhanced photocatalytic hydrogen evolution. *Appl. Catal., B* **2020**, 268, No. 118382.
- (100) Wang, K.; Wang, Q.; Zhang, K.; Wang, G.; Wang, H. Selective solar-driven CO reduction mediated by 2D/2D Bi₂O₃/SiO₂/MXene nanosheets heterojunction. *J. Mater. Sci. Technol.* **2022**, 124, 202–208.
- (101) Madi, M.; Tahir, M.; Zakaria, Z. Y. 2D/2D V₂C mediated porous g-C₃N₄ heterojunction with the role of monolayer/multilayer MAX/MXene structures for stimulating photocatalytic CO₂ reduction to fuels. *J. CO₂ Util.* **2022**, 65, No. 102238.
- (102) Cai, T.; Wang, L.; Liu, Y.; Zhang, S.; Dong, W.; Chen, H.; Yi, X.; Yuan, J.; Xia, X.; Liu, C.; et al. Ag₃PO₄/Ti₃C₂ MXene interface materials as a Schottky catalyst with enhanced photocatalytic activities and anti-photocorrosion performance. *Appl. Catal., B* **2018**, 239, 545–554.
- (103) Qin, J.; Hu, X.; Li, X.; Yin, Z.; Liu, B.; Lam, K.-h. 0D/2D AgInS₂/MXene Z-scheme heterojunction nanosheets for improved ammonia photosynthesis of N₂. *Nano Energy* **2019**, 61, 27–35.
- (104) Wang, H.; Zhao, R.; Qin, J.; Hu, H.; Fan, X.; Cao, X.; Wang, D. MIL-100(Fe)/Ti₃C₂ MXene as a Schottky Catalyst with Enhanced Photocatalytic Oxidation for Nitrogen Fixation Activities. *ACS Appl. Mater. Interfaces* **2019**, 11, 44249–44262.
- (105) Lakhani, M. N.; Hanan, A.; Wang, Y.; Lee, H. K.; Arandiyani, H. Integrated MXene and metal oxide electrocatalysts for the oxygen evolution reaction: synthesis, mechanisms, and advances. *Chem. Sci.* **2024**, 15, 15540–15564.
- (106) Tyndall, D.; Gannon, L.; Hughes, L.; Carolan, J.; Pinilla, S.; Jaśkaniec, S.; Spurling, D.; Ronan, O.; McGuinness, C.; McEvoy, N.; et al. Understanding the effect of MXene in a TMO/MXene hybrid catalyst for the oxygen evolution reaction. *Npj 2D Mater. Appl.* **2023**, 7, 15.
- (107) Wei, J.; Zhou, M.; Long, A.; Xue, Y.; Liao, H.; Wei, C.; Xu, Z. Heterostructured Electrocatalysts for Hydrogen Evolution Reaction Under Alkaline Conditions. *Nanomicro Lett.* **2018**, 10, 75.
- (108) Saini, A.; Yerbulekova, A.; Das, C.; Kharwar, Y. P.; Wertz, A.; Majumder, P.; Shafaat, H. S.; Dutta, A. Designed Metalloprotein-Driven Electrolyzer Operational in Seawater. *ACS Catal.* **2025**, 15, 2620–2629.
- (109) Bai, X.; Guan, J. MXenes for electrocatalysis applications: Modification and hybridization. *Chin. J. Catal.* **2022**, 43, 2057–2090.
- (110) Zubair, M.; Ul Hassan, M. M.; Mehran, M. T.; Baig, M. M.; Hussain, S.; Shahzad, F. 2D MXenes and their heterostructures for HER, OER and overall water splitting: A review. *Int. J. Hydrogen Energy* **2022**, 47, 2794–2818.

- (111) Peera, S. G.; Liu, C.; Sahu, A. K.; Selvaraj, M.; Rao, M. C.; Lee, T. G.; Koutavarapu, R.; Shim, J.; Singh, L. Recent Advances on MXene-Based Electrocatalysts toward Oxygen Reduction Reaction: A Focused Review. *Adv. Mater. Interfaces* **2021**, 8, No. 2100975.
- (112) Pranada, E.; Ngozichukwu, B.; Yoo, R.; Johnson, D.; Barteau, M. A.; Abdel-Wahab, A.; Djire, A. Hydrogen Evolution and Oxygen Reduction on OH/F-Terminated Titanium Nitride MXene Reveal the Role of the Surface Termination Group in Electrocatalysis. *ACS Catal.* **2025**, 15, 982–991.
- (113) Feng, L.; Zha, X.-H.; Luo, K.; Huang, Q.; He, J.; Liu, Y.; Deng, W.; Du, S. Structures and Mechanical and Electronic Properties of the Ti_2CO_2 MXene Incorporated with Neighboring Elements (Sc, V, B and N). *J. Electron. Mater.* **2017**, 46, 2460–2466.
- (114) Xu, J.; Zhou, Z.; Yang, T.; Liu, X.; Tang, G.; Wu, H.; Zhang, D.; Su, Y.; Wu, Z.; Pei, Z.; et al. MXene-Based Oxygen Electrocatalysts: Mechanistic Insights, Property Tuning Strategies, and Prospects toward Practical Applications *Adv. Mater.* **2025**, 37, No. e12724.
- (115) Lei, Z.; Ali, S.; Sathish, C. I.; Ahmed, M.; Qu, J.; Zheng, R.; Xi, S.; Yu, X.; Breese, M. B. H.; Liu, C.; et al. Transition Metal Carbonitride MXenes Anchored with Pt Sub-Nanometer Clusters to Achieve High-Performance Hydrogen Evolution Reaction at All pH Range. *Nanomicro Lett* **2025**, 17, 123.
- (116) Wyatt, B. C.; Rosenkranz, A.; Anasori, B. 2D MXenes: Tunable Mechanical and Tribological Properties. *Adv. Mater.* **2021**, 33, No. 2007973.
- (117) Zhou, S.; Yang, X.; Pei, W.; Liu, N.; Zhao, J. Heterostructures of MXenes and N-doped graphene as highly active bifunctional electrocatalysts. *Nanoscale* **2018**, 10, 10876–10883.
- (118) Cheng, C.; Zhang, X.; Fu, Z.; Yang, Z. Strong metal–support interactions impart activity in the oxygen reduction reaction: Au monolayer on Mo_2C (MXene). *J. Phys.: Condens. Matter* **2018**, 30, No. 475201.
- (119) Dhakshinamoorthy, A.; Ramírez-Grau, R.; Garcia, H.; Primo, A. Opportunities of MXenes in Heterogeneous Catalysis: V_2C as Aerobic Oxidation Catalyst. *Chem. Eur. J.* **2024**, 30, No. e202400576.
- (120) Liu, B.; Chen, H.; Zhao, C.; Liang, H. EGCG mildly reduced single atom Co-MXene catalytic membrane: Catalytic and antioxidant properties. *Chem. Eng. J.* **2024**, 499, No. 156416.
- (121) Li, K.; Jiao, T.; Xing, R.; Zou, G.; Zhao, Q.; Zhou, J.; Zhang, L.; Peng, Q. Fabrication of hierarchical MXene-based AuNPs-containing core–shell nanocomposites for high efficient catalysts. *Green Energy Environ.* **2018**, 3, 147–155.
- (122) Slot, T. K.; Natu, V.; Ramos-Fernandez, E. V.; Sepúlveda-Escribano, A.; Barsoum, M.; Rothenberg, G.; Shiju, N. R. Enhancing catalytic epoxide ring-opening selectivity using surface-modified $\text{Ti}_3\text{C}_2\text{T}_x$ MXenes. *2D Mater.* **2021**, 8, No. 035003.
- (123) Li, Z.; Yu, L.; Milligan, C.; Ma, T.; Zhou, L.; Cui, Y.; Qi, Z.; Libretto, N.; Xu, B.; Luo, J.; et al. Two-dimensional transition metal carbides as supports for tuning the chemistry of catalytic nanoparticles. *Nat. Commun.* **2018**, 9, No. 5258.
- (124) Vohra, M. I.; Alasiri, A.; Ateeq, M.; Sakr, R. Y.; Krzywiecki, M.; Shehzad, K.; Azizi, S.; Zada, A. Coordination between semiconductor defects and their role in charge separation and light absorption for exceptional solar light driven photocatalysis. *Coord. Chem. Rev.* **2025**, 545, No. 217017.
- (125) Sun, Y.; Jin, D.; Sun, Y.; Meng, X.; Gao, Y.; Dall'Agnese, Y.; Chen, G.; Wang, X.-F. $\text{g-C}_3\text{N}_4/\text{Ti}_3\text{C}_2\text{T}_x$ (MXenes) composite with oxidized surface groups for efficient photocatalytic hydrogen evolution. *J. Mater. Chem. A* **2018**, 6, 9124–9131.
- (126) Misra, M.; Sreedhar, A.; Noh, J.-S. Advancements in 2D Ti_3C_2 MXene interfaced various metal oxide semiconductors for photo-electrochemical water splitting: A review. *Microchem. J.* **2025**, 216, No. 114632.
- (127) Emmanuel, S. S.; Adesibikan, A. A.; Tichapondwa, S. M.; Rayaroth, M. P.; Bosca, F.; Marin, M. L.; Samejo, B. A.; Boczkaj, G. MXenes as sustainable functional nanomaterials for photocatalytic degradation of dye pollutants: Performance, effect of process parameters, stability and re-useability evaluation – A critical review. *Sustain. Mater. Technol.* **2025**, 46, No. e01683.
- (128) Hassan, N. S.; Jalil, A. A.; Bahari, M. B.; Izzuddin, N. M.; Fauzi, N. A. F. M.; Jusoh, N. W. C.; Kamaroddin, M. F. A.; Saravanan, R.; Tehubijuluw, H. A critical review of MXene-based composites in the adsorptive and photocatalysis of hexavalent chromium removal from industrial wastewater. *Environ. Res.* **2024**, 259, No. 119584.