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MXene–MOF Hybrid Nanocomposites: Emerging Platforms for Sustainable Wastewater Treatment

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ABSTRACT

The rapid increase in the discharge of chemically complex wastewater, driven by urbanization, industrial intensification, and technological expansion, continues to exceed the capacity of conventional wastewater treatment infrastructure. This undermines progress toward Sustainable Development Goal 6, particularly Target 6.3, which aims to reduce untreated wastewater discharge by 50% by 2030. Addressing this challenge necessitates the development of material platforms capable of selective, high-efficiency, and multi-contaminant removal under realistic operating conditions. Metal–organic framework (MOF)–MXene hybrid nanocomposites have recently emerged as promising functional materials for advanced wastewater remediation applications. These materials integrate the high surface area and tunable porosity of MOFs with the electrical conductivity, hydrophilicity, and surface functionality of MXenes. The resulting synergistic architectures facilitate enhanced adsorption, catalytic degradation, and redox-mediated removal of a broad spectrum of pollutants. Although original research articles account for the majority of publications in this field (85%), comprehensive review articles remain limited (8%), indicating a clear knowledge gap in the literature. Therefore, this review critically discusses recent advances in MXene–MOF hybrid nanocomposites for wastewater treatment, with an emphasis on their design and synthesis strategies, pollutant removal mechanisms, and the key challenges that must be addressed for practical implementation of these materials.

1 | Introduction

Sustainable Development Goal 6 (SDG 6), established by the United Nations (UN), aims to ensure universal access to clean water and sanitation by 2030. Among its targets, SDG 6.3 specifically aims to improve water quality by reducing pollution, eliminating dumping, minimizing the release of hazardous

chemicals, halving the proportion of untreated wastewater, and substantially increasing recycling and the safe reuse of water worldwide. The progress toward this target is monitored through two primary indicators: (i) the proportion of domestic and industrial wastewater flows safely treated (6.3.1), and (ii) the proportion of water bodies meeting good ambient water quality standards (6.3.2).

Kalaimani Markandan and Theeba Rajasegran are equal first author to this study.

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The 2024 UN-Water progress report for indicator 6.3.2 revealed that the water quality of many surface and groundwater bodies remains below acceptable standards, with only a subset of water bodies meeting the “good quality” criteria in 2023 relative to 2017 [1]. Regions such as Oceania, Australia, and New Zealand have a high number of rivers and lakes with satisfactory water qualities. Figure 1 shows that regions such as sub-Saharan Africa, Latin America, and Central and Southern Asia experience a significant occurrence of water bodies with low quality. Rivers in these areas are notably affected by the ongoing discharge of industrial waste and agricultural runoffs. Although governance policies and monitoring initiatives are in place, the minimal temporal improvement in ambient water quality highlights the challenges of effectively managing water pollution. This highlights the shortcomings of conventional methods, such

as biological treatment, coagulation–flocculation, and filtration, in effectively eliminating persistent organic compounds, pharmaceuticals, heavy metals, antibiotics, endocrine disruptors, and other emerging pollutants, including per- and polyfluoroalkyl substances (PFAS).

Therefore, materials that are effective in removing contaminants and meet stringent regulatory requirements are in high demand. Nanostructured materials, specifically hybrids of metal–organic frameworks (MOFs) and MXenes, have been recognized as promising candidates for advanced wastewater treatment. The standalone application of MXenes has been hindered by oxidation and restacking, whereas MOFs experience hydrolytic instability and leaching of metal ions [2]. The formation of MXene–MOF heterostructures alleviates the limitations

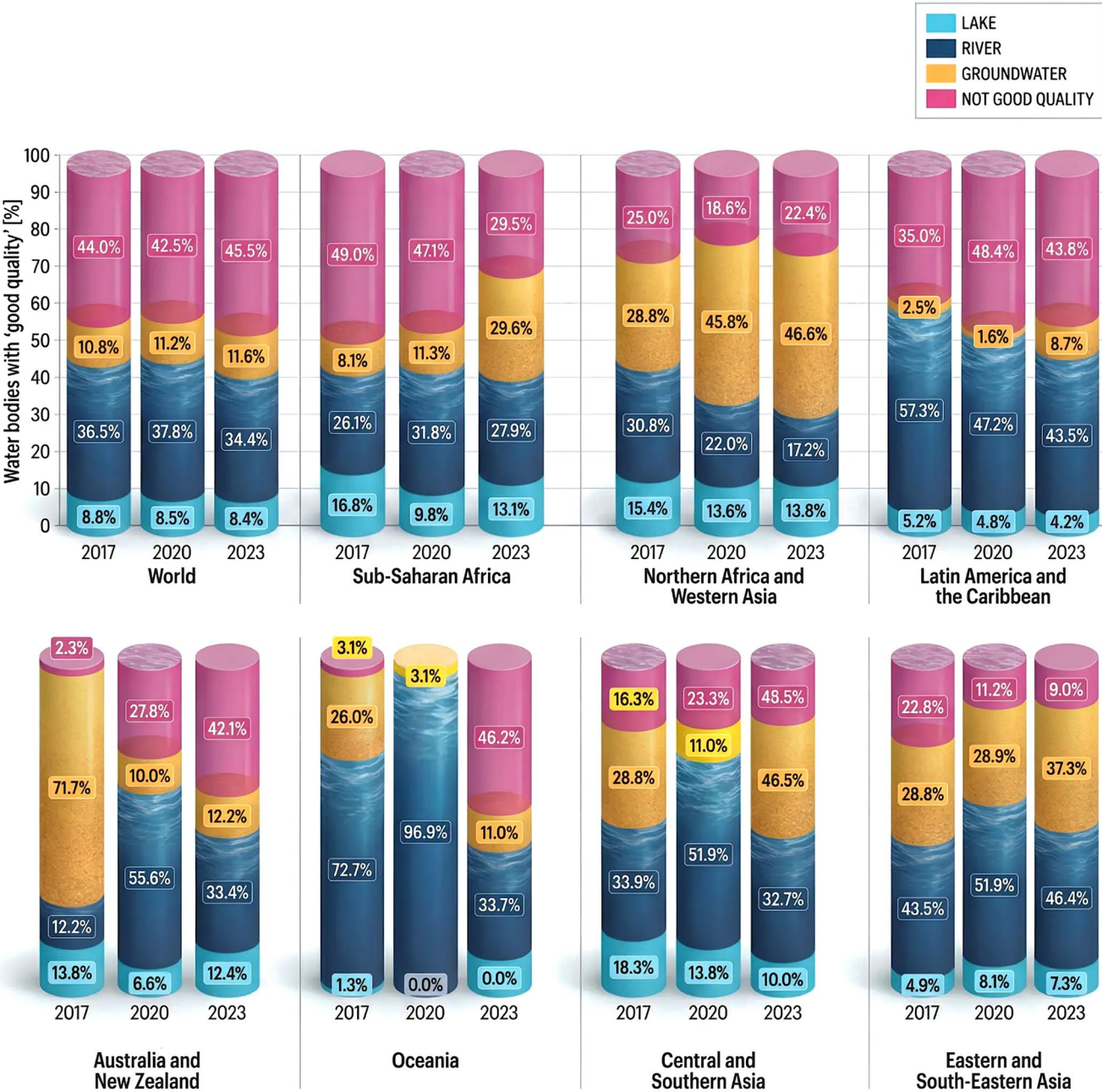


FIGURE 1 | Proportion of water bodies with good ambient water quality in various regions. Adapted from the UN-Water SDG Indicator 6.3.2 Progress Report (2024).

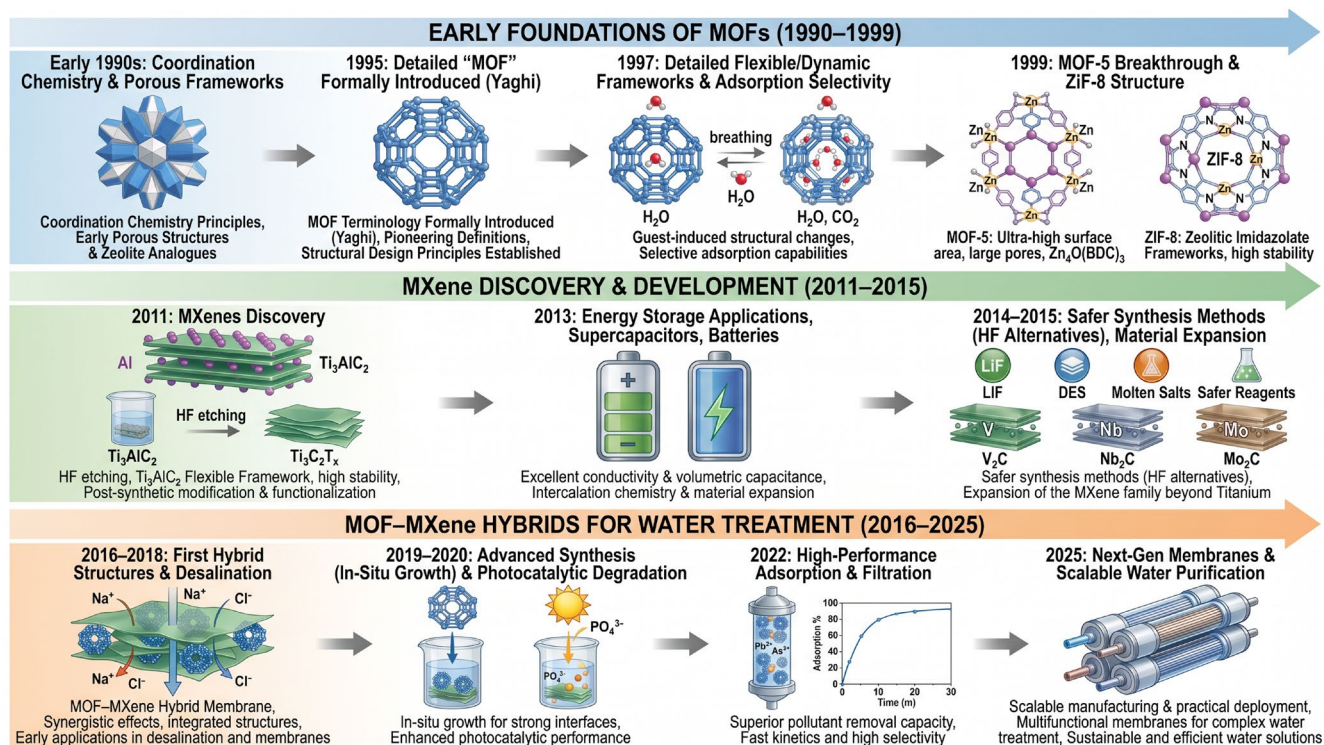


FIGURE 2 | Timeline illustrating the evolution of MOFs, MXenes, and MOF-MXene hybrids.

of MOFs. MXenes have high intrinsic electrical conductivity, hydrophilic surfaces, and abundant terminal functional groups, which promote strong coordination with metal ions and organic contaminants while facilitating rapid electron transfer during catalytic reactions [3, 4]. MOFs also provide exceptionally high surface areas, well-defined pore architectures, and tunable metal-ligand coordination environments that enable the selective adsorption and efficient catalytic transformation of hazardous species [5].

Several studies have demonstrated the efficacy of MOF-MXene composites in water remediation. Far et al. [3] reported that $\text{Ti}_3\text{C}_2\text{T}_x$ MXene hybridized with a zirconium-based MOF (UiO-66) achieved high dye removal efficiencies of 88.95% for methyl orange and 76.98% for Direct Red 31, with sustained stability and reusability over four adsorption-desorption cycles. Similarly, Najibikhah et al. [6] demonstrated that Ni-MOF/ $\text{Ti}_3\text{C}_2\text{T}_x$ composites with a specific surface area of $25.3 \text{ m}^2 \text{ g}^{-1}$ reached a maximum adsorption capacity of $1012.37 \text{ mg g}^{-1}$ for methylene blue, attributed to enhanced electrostatic interactions, π - π stacking, and hydrogen bonding. Recently, Zhang et al. [7] reported that ZnBDC-NH_2 MOF nanosheets integrated with negatively charged MXene exhibited exceptional antibiotic-desalination performance, achieving 97.59% chloramphenicol rejection with an unprecedented water permeance of $269.3 \text{ L m}^{-2} \text{ h}^{-1} \text{ bar}^{-1}$ and operational stability exceeding 120 h. Notably, the reported water permeance is five- to tenfold higher than that of previously reported membranes with comparable antibiotic rejection.

Figure 2 shows the chronological progression of MOFs, MXenes, and their subsequent integration into MOF-MXene hybrid systems. This developmental timeline began with the groundbreaking

work of Yaghi and co-workers in 1995, which introduced MOFs as a distinct class of crystalline porous coordination polymers. This was followed by the synthesis of MOF-5 in 1999, a pioneering example of a highly porous and structurally stable MOF that established the feasibility of rational framework design. Subsequent advances led to the development of isorecticular MOFs (IRMOFs), which enabled systematic tuning of pore size and functionality based on the principles of reticular chemistry. The introduction of MIL-101(Cr) in 2005 marked a further milestone in MOF research, owing to its exceptionally high surface area and large pore volume, which broadened both the structural diversity and potential applications of MOFs [8–11]. Collectively, these innovations have positioned MOFs as versatile platforms for applications in gas storage, catalysis, and separation technologies. A pivotal moment occurred in 2011 with the discovery of MXenes by Naguib et al. These materials, derived from layered MAX phases through selective etching, are two-dimensional transition metal carbides and nitrides known for their high electrical conductivity, hydrophilicity, and adaptable surface chemistries. Their effectiveness as electrodes in high-rate lithium-ion batteries was rapidly demonstrated, emphasizing their potential for electrochemical energy storage [12, 13]. Recognizing the complementary properties of MOFs (notably high porosity and structural adaptability) and MXenes (notably electrical conductivity and mechanical strength), MOF-MXene hybrid systems have emerged since 2018. These composites capitalize on the strengths of both components, leading to enhanced performance in various applications. Initial research focused on energy storage, where the hybrids showed improved electrical conductivity and ion-transport kinetics. Their range of applications has rapidly expanded to include electrocatalysis [14, 15], gas separation [16], and flexible sensing platforms for wearable electronics [17]. The graphical timeline further contextualizes the rapid evolution of MOFs, MXenes, and MOF-MXene hybrids for various engineering applications.

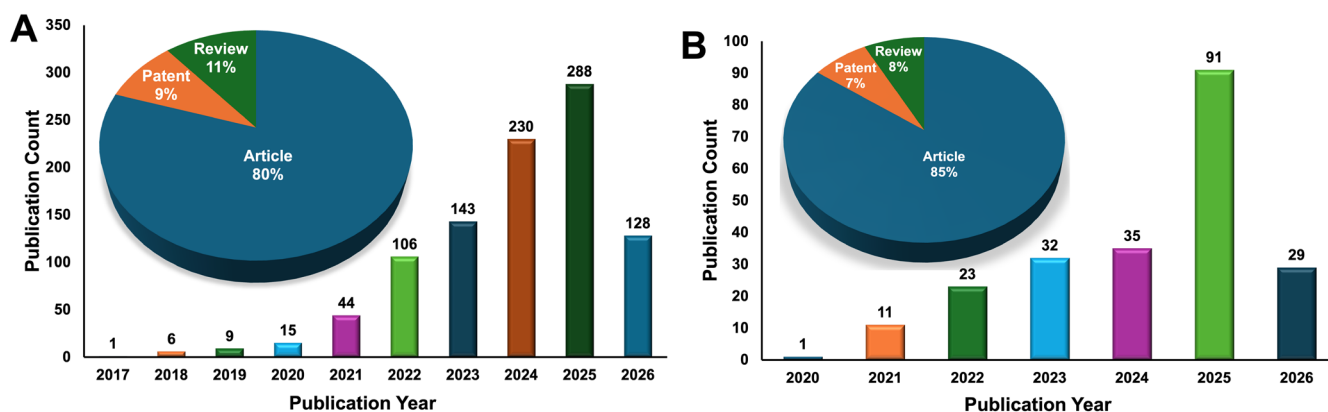


FIGURE 3 | (A) Number of publications on MOF-MXene composites; (B) Publications on MOF-MXene composites in water treatment; inset shows the publication breakdown (Data from Web of Science, accessed on April 26, 2026).

Despite their promising physicochemical properties, including combined micro/mesoporosity, enhanced electrical conductivity, mechanical robustness, and tunable surface chemistry, dedicated review articles critically examining MOF-MXene composite applications in the treatment of hazardous wastewater remain conspicuously limited. A systematic search of the Web of Science database spanning 2015 to 2026 reveals a pronounced and sustained increase in publications concerning MXene-MOF composites, confirming that this hybrid material class has rapidly emerged as a focal point of environmental remediation research.

Figure 3A illustrates that the number of publications on MXene-MOF composites was minimal before 2018. However, there was a progressive increase in output thereafter, with a significant acceleration from 2021 onwards. This trend aligns with the broader development of scalable MXene synthesis protocols and the simultaneous diversification of MOF structural platforms. Figure 3B further indicates that, while the use of MXene-MOF hybrids in water treatment has significantly expanded during the same period, the literature is predominantly composed of original research articles (85%), with reviews constituting only 8% and patents 7% of the total output. This distribution of document types is significant for interpretation: the predominance of primary research over comprehensive synthesis suggests a field still in an active phase of knowledge generation, where the experimental scope is expanding more rapidly than critical consolidation.

The dominance of original research over integrative review articles highlights a significant gap in comprehensive critical analysis, especially concerning performance trade-offs, the reproducibility of mechanisms, and the comparability of studies. A common issue in primary research is the presentation of extremely high adsorption capacities and degradation efficiencies achieved under ideal laboratory conditions. These conditions often involve single-contaminant systems, buffered model solutions, and optimized contact times, which do not accurately reflect the chemical complexities of real wastewater. These environments are characterized by competing ionic species, natural organic matter, varying pH levels, and fluctuating contaminant loads. Consequently, the translation gap between bench-scale performance and real-world applicability remains inadequately addressed, and the field lacks the rigorous

comparative frameworks needed to evaluate scalability, long-term operational stability, and regeneration feasibility across diverse system configurations.

In this context, the present review aims to provide a critical and comparative examination of MXene-MOF hybrid nanocomposites for the treatment of hazardous wastewater. Specifically, it addresses three interconnected dimensions: (i) the principal design philosophies and synthesis strategies governing hybrid fabrication, including in situ growth, electrostatic self-assembly, and covalent surface functionalization; (ii) the mechanistic underpinnings of pollutant removal, encompassing adsorption, heterogeneous photocatalysis, and ion exchange, with particular attention to structure-performance relationships; and (iii) the practical challenges and inherent trade-offs associated with real-world deployment, including material scalability, regeneration efficiency, and stability under operationally relevant conditions, alongside a prospective assessment of the directions most likely to bridge the current gap between laboratory promise and applied environmental technology.

2 | Design and Synthesis of MXene-MOF Hybrids

2.1 | Synthetic Strategies

2.1.1 | Direct Synthesis

Ti₃C₂T_x is the most extensively studied MXene material because of its facile synthesis, high yield, relative chemical stability, and desirable physicochemical properties. It is typically synthesized via selective etching of the Ti₃AlC₂ MAX phase using hydrofluoric acid (HF) or in situ HF-generating fluoride salt/acid mixtures (e.g., LiF/HCl), followed by chemical intercalation and mechanical exfoliation to obtain individual sheets. The resulting single- or few-layer MXene sheets, with large lateral dimensions and high aspect ratios obtained from the delamination step, are critical for the subsequent formation of hybrid structures. In addition, the synthesis conditions affect the structural order, defect density, and surface chemistry, wherein etchant composition, temperature, and intercalants control the type and density of surface terminations (-O, -OH, -F, -Cl). These characteristics influence dispersibility, colloidal stability, and interfacial

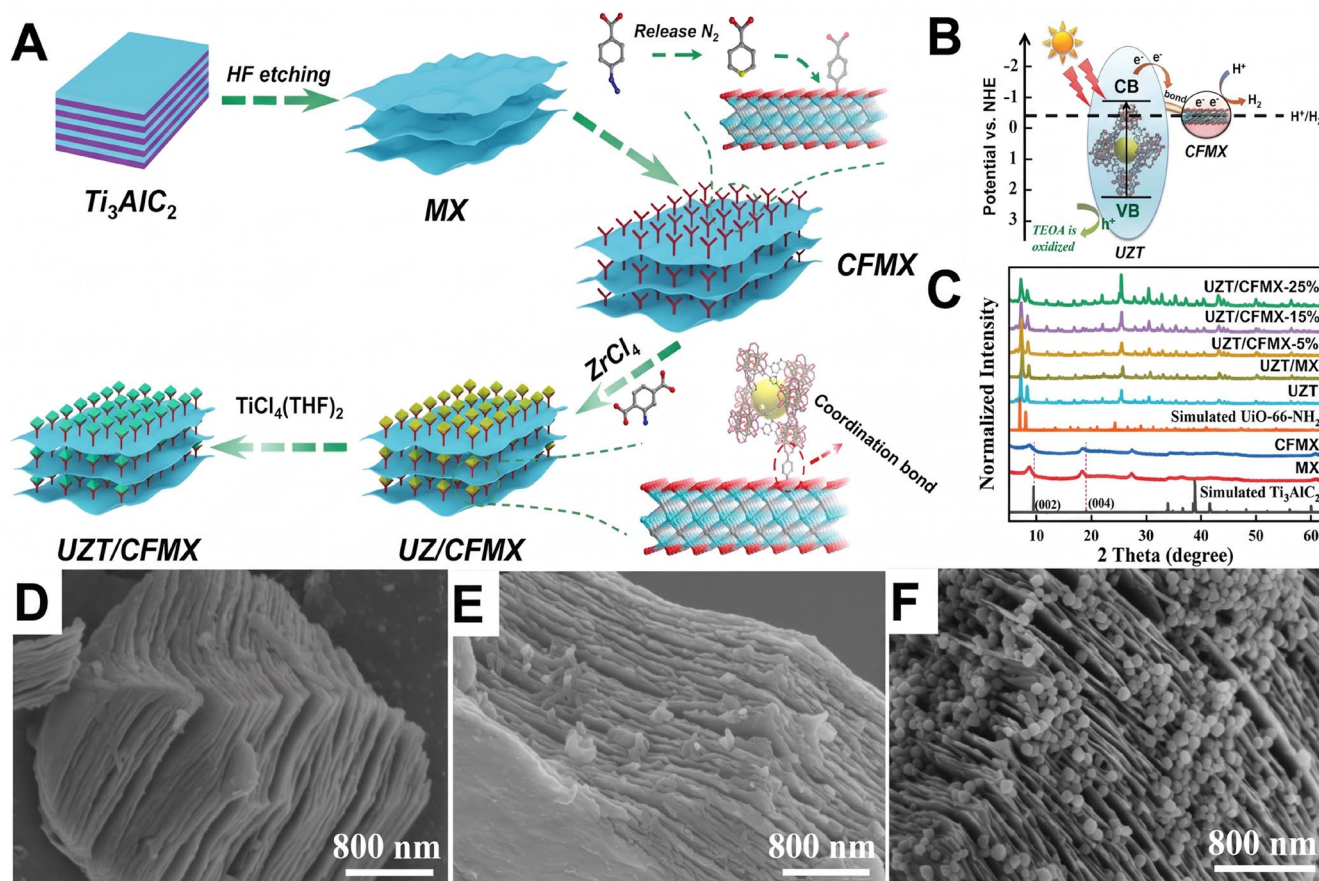


FIGURE 4 | (A) Schematic representation for formation of carboxyl-functionalized MXene (CFMX) and growth of UZT on surface of MXene (CFMX) (B) Water splitting by photocatalysis of MXene–MOF hybrid with improved interfacial charge transfer after functionalization (C) XRD patterns of Ti_3AlC_2 , MXene, CFMX, MOF and MXene–MOF hybrid. SEM images of (D–F) MXene, CFMX, and MXene–MOF hybrid, showing the layered structure and homogenous MOF dispersion on MXene sheets. Adapted from [23] with permission from Wiley.

interactions with MOF precursors during hybrid assembly [18]. The controlled tuning of MXene behavior, such as surface chemistry, electronic structure, and morphology, further promotes efficient MOF nucleation and stable composite formation [19].

2.1.2 | Ex-Situ Assembly and Physical Hybridization

In the ex-situ assembly, MXene nanosheets and MOF particles are synthesized separately to preserve their intrinsic structural characteristics prior to hybridization and are subsequently integrated into a common medium. Assembly is primarily controlled by non-covalent interactions, such as electrostatic attraction, hydrogen bonding, and van der Waals forces, which facilitate spontaneous assembly in solution. Electrostatic interactions between the negative surface charge from the deprotonated –OH terminations of MXenes and positive charge from nitrogen ligand-based MOFs promote rapid self-assembly without harsh reaction conditions or covalent modifications [20, 21].

Most ex-situ methods use solution mixing and subsequent vacuum filtration to fabricate layered films or membranes with adjustable thicknesses and compositions. Sequential deposition techniques with controlled filtration of MXenes and MOFs facilitate the formation of multilayer or sandwich-type architectures to intentionally control the interlayer spacing, mechanical

integrity, and mass transport pathways for catalytic and separation applications [21]. The advantage of ex situ hybridization is that it proceeds under mild conditions, which minimizes process complexity and is compatible with scalable manufacturing [22].

Figure 4 illustrates the direct ex situ formation of the MXene–MOF heterostructure designed for solar-driven photocatalytic water splitting, wherein UiO-66-NH₂(Zr/Ti) was coupled with carboxyl-functionalized MXene. The functional groups provide coordination sites that promote interfacial interactions and enhance interfacial charge transport, thereby improving the photocatalytic performance [23].

Despite its practical advantages, ex situ hybridization is limited by weak chemical bonding at the MXene–MOF interface, which can compromise mechanical stability, hinder interfacial charge transfer, and lead to performance degradation during long-term operation. In addition, non-uniform dispersion of MOF particles on MXene sheets can limit the utilization of active sites [24]. Consequently, although physical hybridization often yields synergistic improvements relative to the individual constituents, its functional efficiency remains lower than that of chemically integrated synthetic routes.

Nonetheless, ex-situ assembly remains advantageous for screening, preliminary studies, and scale-up applications, where the

simplicity of the synthesis route outweighs the need for strong interfacial bonding. This method also offers key insights into electrostatic assembly mechanisms and morphological compatibility of MXene–MOF hybrids to guide the design of more advanced hybridization strategies [25].

2.1.3 | In Situ Growth and Interfacial Engineering

In situ growth is an effective strategy for synthesizing MXene–MOF nanocomposites with enhanced interfacial bonding and improved synergistic properties, in which MOFs nucleate and grow directly on the MXene surface, resulting in stronger interfacial adhesion and improved structural stability [24]. The effectiveness of in situ hybridization depends on the surface chemistry of MXenes, where the –OH and –O surface terminations serve as metal–ion binding sites to facilitate controlled MOF formation [26]. Advanced ionothermal synthesis has facilitated direct coordination bonding between MXenes and MOFs to produce heterointerfaces with enhanced mechanical strength and electrical properties. Here, MXene sheets function as templates that allow oriented MOF growth and porous structures that are either hierarchical or vertically aligned [27].

In contrast to ex-situ methods, in situ hybrids exhibit stronger interfacial interactions and superior functional performance [28]. However, in situ synthesis techniques are constrained by several limitations. For instance, synthesizing MOFs requires extended processing times, elevated temperatures, and inert conditions, resulting in increased energy consumption and production expenses. Additionally, harsh synthesis conditions can compromise the structural integrity of MXenes. Consequently, achieving uniform MOF deposition without affecting the MXene structure is challenging, particularly at a large scale. Overall, in situ growth combined with interfacial engineering offers an effective, albeit complex, approach for fabricating MXene–MOF hybrids that are suitable for practical wastewater treatment applications [29].

2.1.4 | Other Innovative Strategies

In addition to conventional ex-situ and in situ growth methods, several advanced synthesis techniques have been reported to produce MXene–MOF hybrids with strong interfaces and device adaptability. These include electrochemical deposition, microwave-assisted synthesis, additive manufacturing, and sequential deposition [30].

Electrochemical deposition is a fast and effective technique for synthesizing MXene–MOF composite films directly onto conductive supports using an electric potential applied to an electrolyte containing exfoliated MXene nanosheets, metal ions (e.g., Ni^{2+} , Co^{2+} , $\text{Fe}^{2+}/\text{Fe}^{3+}$, Cu^{2+} , or Zn^{2+}), and organic linkers (e.g., 2-methylimidazole, trimesic acid, or terephthalic acid). The applied electric potential alters the pH as well as redox reactions at electrode surface for MOF formation while ensuring the positioning of MXene sheets in the composite [18]. The one-step electrochemical route enables controlled fabrication of the coating by adjusting applied voltage, deposition time, electrolyte

concentration and scanning mode (i.e., potentiostatic or galvanostatic) [31]. However, the applicability of this technique is limited by several factors, including the requirement for conductive substrates, nonuniform deposition over large areas, scale-up challenges arising from electrode-size restrictions, and mass-transport resistance within thick films.

Microwave-assisted synthesis enables the rapid production of MXene–MOF hybrids, in which microwave irradiation provides uniform volumetric heating through dipolar polarization and ionic conduction, thereby significantly reducing the synthesis time from hours to minutes. In a typical process, MXene suspensions are combined with metal ions (such as Zr^{4+} for UiO-type MOFs, Cu^{2+} for HKUST-1, and Fe^{3+} for MIL-series MOFs) and organic linkers. Rapid heating promotes homogeneous nucleation and controlled growth of MOF crystals on MXene sheets to prevent particle agglomeration. The main advantage of this technique is the production of MXene–MOF hybrids with a uniform structure, high crystallinity, and narrow particle size distribution. In addition, rapid reaction prevents the oxidation of MXenes while reducing energy consumption relative to conventional solvothermal methods and is compatible with diverse MOF chemistries and solvents [32]. Careful control of microwave parameters is essential to prevent overheating, which can lead to MXene degradation or nonuniform MOF formation. It should also be noted that the reactor volume and penetration depth of microwave irradiation can constrain scalability, which hinders industrial applications.

Additive manufacturing is an advanced strategy for fabricating MXene–MOF composites, offering unprecedented structural and functional control. Printable inks are prepared by blending MXene flakes with MOF precursors/preformed particles and rheological modifiers or polymeric binders (e.g., polyvinylpyrrolidone, polyethylene oxide, or alginate). These inks allow the fabrication of self-standing architectures, such as lattices, scaffolds, and porous monoliths, using various techniques, including extrusion-based printing, direct ink writing, and robocasting. Subsequent post-printing treatments, such as solvothermal crystallization, thermal activation, or ligand exchange, are used to produce MOFs or improve the structural crystallinity within the MXene framework [33]. This method offers precise control over the structural geometry, pore distribution, and functional gradients, which are crucial for applications such as sensors, flow reactors and membranes [34]. Figure 5 shows the characterization of 3D-printed MXene–MOF composites for the adsorptive removal of dyes from wastewater, where the hybrid structure was attached to a hierarchically porous 3D-printed lattice for mechanical support (Figure 5A). The FESEM images reveal that the 3D-printed lattice had macroscopic channels with uniform spacing (Figure 5B,C) for facile liquid flow and reduced diffusion resistance during adsorption. High-magnification images also reveal that ZIF-8 crystals were uniformly distributed within the MXene layers (Figure 5C). The FTIR spectra in Figure 5D show the characteristic vibrational bands and stretching modes of MXene and MOF, confirming their incorporation into the hybrid material. The 3D-printed composite also maintained removal efficiency after repeated adsorption and desorption cycles, highlighting the reusability of the composite [35]. However, the binders used can affect

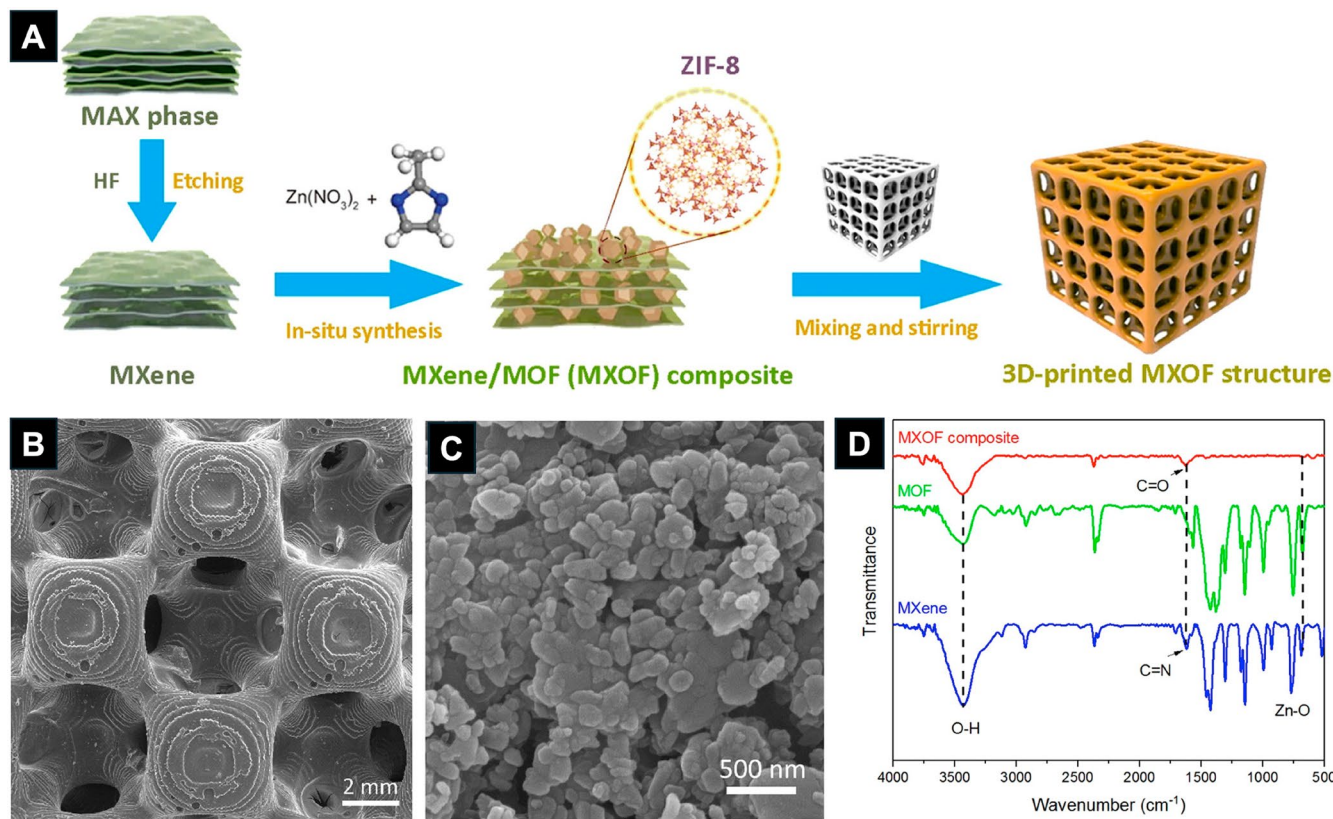


FIGURE 5 | (A) MXene–MOF hybrid fabricated via 3D printing by immobilization on a porous lattice scaffold. (B, C) FESEM images of the 3D-printed lattice at different magnifications, showing the macroscopic channels and coverage of MXene–MOF on the lattice surface. (D) FTIR spectra of MXene, MOF, and MXene–MOF composite. Adapted with permission from [35] ACS Publications.

the electrical conductivity and limit the availability of active sites, whereas post-printing processes might cause shrinkage or fracturing of the structure. Therefore, optimizing printability without compromising structural integrity and functional performance is important.

Sequential deposition (layer-by-layer assembly) allows synthesis of MXene–MOF hybrids with tunable multilayer architectures; via sequential deposition of MXene layers and MOF precursor solutions using techniques such as dip coating, spin coating, spray coating, or Langmuir–Blodgett assembly. The thickness increased in a controlled manner for every cycle to ensure accurate control of the interfacial density and mass transport pathways, while preventing MXene agglomeration and ensuring homogeneous MOF coverage [36]. Despite these advantages, the multistep process can be slow, and poor interfacial adhesion can hinder efficient mass transfer and catalytic performance [37]. Table 1 summarizes MXene–MOF hybrids and their synthesis methods for wastewater treatment applications. The trade-offs highlight that improved structural integration does not always translate into superior functional performance, particularly under continuous operation conditions.

2.2 | Structural and Functional Integration

MXene–MOF hybrids integrate the functional characteristic of each constituent into one structure. MXenes impart high electrical conductivity, hydrophilicity, and surface functionality,

whereas MOFs provide adjustable porosity and active metal sites with selective adsorption. Therefore, MXene–MOF composites allow faster ion and electron transport with higher structural stability and multifunctional operation for effective wastewater treatment. This section discusses the functionalities of MXenes and MOFs, as well as the synergistic effect of MXene–MOF hybrids on enhancing composite performance.

2.2.1 | MXenes Functionality

MXenes exhibit metallic or semi-metallic conductivity exceeding 10000 Scm^{-1} , which facilitates efficient electron transfer in hybrid materials. When integrated with insulating MOFs, MXenes provide conductive pathways that improve charge transport for electrochemical applications, such as pollutant degradation, energy storage, and electrocatalysis. In MXene@ZIF-8 composites, electrons produced at active sites of MOF are effectively transported through the MXene framework to improve the overall electrochemical performance. In addition, MXenes exhibit excellent hydrophilicity owing to the surface terminations ($-\text{OH}$, $-\text{O}$, $-\text{F}$, and $-\text{Cl}$) introduced during HF or LiF/HCl etching. The hydrophilic behavior of MXene–MOFs improves their interactions with water and promotes the rapid diffusion of aqueous molecules into the structure. In membranes, adsorption, and water purification applications, efficient mass transfer and enhanced water compatibility are essential for optimal pollutant removal. In these cases, MXene terminations function as anchoring sites for MOF nucleation.

TABLE 1 | Summary of MXene–MOF hybrids based on their synthesis methods and morphologies for wastewater treatment applications.

MOF material	Mxene material	Synthesis method	Morphology	Application	Primary application	References
UiO-66-NH ₂ (Zr/Ti)	Carboxyl-functionalized Ti ₃ C ₂ T _x	Carboxyl-assisted coordination bonding between MOF nodes and surface-grafted carboxyl groups on MXene	Well-coupled heterostructure with MOF particles homogenously deposited on 2D MXene sheets (2D–3D heterointerface)	Photocatalytic water splitting for H ₂ production	Hydrogen evolution reaction	[23]
Porous covalent organic framework (COF) nanosheets	Ti ₃ C ₂ T _x	Layer-by-layer membrane assembly i.e., dual-layer deposition via vacuum assisted	Bilayer laminated structure with ~8 nm ultrathin MXene film deposited on porous COF layer	Membrane-based water treatment (dye separation)	Wastewater treatment	[36]
ZIF-8 (Zn-based MOF) nanoparticles	Ti ₃ C ₂ T _x	Ex situ insertion of nanoparticles between layers by physical intercalation	2D–3D interlayer hybrid; ZIF-8 nanoparticles embedded between MXene sheets	Removal of organic methylene blue dyes via adsorption	Wastewater treatment	[38]
Tannic acid–modified ZIF-8 (TA–ZIF-8)	Ti ₃ C ₂ T _x	Membrane formation via vacuum filtration using modified MOF nanoparticles	Laminated MXene membrane embedded with MOF nanoparticles; mixed-dimensional (2D MXene–3D MOF) hierarchical membrane	Treatment of oily wastewater, separation of oil–water emulsion	Wastewater treatment	[39]
ZIF-8 (zeolitic imidazolate framework)	Ti ₃ C ₂ T _x MXene with tailored surface terminations (–O, –OH)	Interlayer MOF integration with modified surface chemistry	2D–3D interlayer hybrid	Removal of organic dyes and antibiotics such as methyl orange, ciprofloxacin via adsorption	Wastewater treatment	[40]
Zn-MOF (ZIF-type)	Ti ₃ C ₂ T _x	3D printing and subsequent post-deposition of MOF	Hierarchical 3D lattice architecture	Removal of anionic dyes such as methyl orange, direct red 31 via adsorption	Wastewater treatment	[35]
Bimetallic ZIF-derived carbon (Co-based ZIF, carbonized)	Ti ₃ C ₂ T _x	Self-assembly followed by thermal carbonization	2D–3D heterojunction architecture	Capacitive deionization (CDI) for seawater desalination	Water desalination	[41]
Tannic acid–modified ZIF-8 (TZIF-8)	Ti ₃ C ₂ T _x	Surface functionalization and dip-coating on stainless-steel mesh	3D stainless-steel mesh	Separation of oil–water	Wastewater treatment	[42]

(Continues)

TABLE 1 | (Continued)

MOF material	Mxene material	Synthesis method	Morphology	Application	Primary application	References
ZIF-67	$\text{Ti}_3\text{C}_2\text{T}_x$	In-situ growth on Sepiolite (Sep) using cross linker (PVP) and later hydrothermally assembled with polydopamine (PDA)	Hierarchically structured membrane composed of MXene/PDA/Sep@ZIF-67 with enhanced hydrophilicity and active-sites	Separation of oil-water	Wastewater treatment	[43]
NiSe ₂	$\text{Ti}_3\text{C}_2\text{T}_x$	In-situ growth of NiSe ₂ octahedral crystals with ultrathin $\text{Ti}_3\text{C}_2\text{T}_x$	Core-shell octahedral structure	Hydrogen evolution reaction	Hydrogen evolution reaction	[44]
ZIF-67	Laminar stacked MXene films (90nm)	Solvothermal growth on Co(II)-MXene modified $\alpha\text{-Al}_2\text{O}_3$ disks	Intergrown membrane (~4 μm thickness)	Gas separation (He/N ₂ , He/CH ₄)	Gas separation	[45]
ZIF-L	$\text{Ti}_3\text{C}_2\text{T}_x$	Composite stacking membrane fabrication	2D-2D layered MXene/ZIF-L hybrid	Dye nanofiltration	Wastewater treatment	[46]
UiO-66-NH2	$\text{Ti}_3\text{C}_2\text{T}_x$	Direct PES membrane synthesis	2D-2D layered	Dye and salt separation	Wastewater treatment	[47]
Bi-ligand ZIF-67	2D MXene	In-situ growth	2D-3D heterojunction	Electrocatalytic water splitting	Hydrogen evolution reaction	[48]

For example, the $-OH$ and $-O$ groups can chelate metal ions, such as Zn^{2+} , Co^{2+} , Ni^{2+} , and Zr^{4+} , from MOF precursors to initiate in situ MOF crystallization.

Surface modification techniques have been reported to further improve these characteristics [49]. For instance, polydopamine or silane coupling agents can introduce $-NH_2$ groups into a molecule, whereas polymer grafting with polyethylene glycol or polyvinylpyrrolidone can prevent restacking and produce more hydrogen-bonding sites. In addition, phytic acid can introduce phosphate groups into high-affinity metal-binding sites that act as nucleation centers for MOF synthesis. These modifications increase the adsorption capacity of MOFs and enable hierarchical porosity with high reaction sites, while the MXene sheets provide a rigid support for MOF growth and prevent collapse. In addition, the 2D lamellar structure of MXenes promotes the intercalation and confinement of MOF crystals to regulate their size, porosity, and orientation. Confinement inhibits the restacking of MXenes to preserve their high surface area and maximize the accessibility of active sites. MXenes also improve electrical conductivity, facilitate mass transport, provide reactive sites, and ensure stability during MOF formation [50]. Collectively, these properties synergistically improve the structural robustness and performance of MXene–MOF hybrids.

2.2.2 | MOF Functionality

The multiscale porosity of MOFs (micro-, meso-, and macropores) provides large internal surfaces for adsorption, catalytic processes, and ion storage applications [51, 52]. By selecting suitable metal nodes or organic linkers, the porous environment can be modified for more selective adsorption based on molecule size, charge, and polarity [53]. For example, ZIF-8, with its cage-like cavities and narrow apertures, is suitable for the adsorption of small organic molecules, whereas MIL-101(Cr), with a Brunauer–Emmett–Teller (BET) surface area of $\sim 4000\text{ m}^2\text{g}^{-1}$ and mesoporous cavities, is well-suited for gas storage and heavy-metal adsorption.

In addition to adsorption, the metal centers in MOFs are reactive sites for redox, photocatalytic, and electrocatalytic reactions. When incorporated with MXenes, electrons move easily at metal sites, which enhances catalytic behavior and prevents aggregation of MOF particles [54]. The structure of MOFs can be altered using linkers, metal ions, or post-synthetic modifications. For example, functional groups such as $-NH_2$, $-COOH$, or $-SO_3H$ can enhance interactions with contaminants or active organisms. The functional groups in MXene–MOF hybrids can establish additional hydrogen bonding or interfacial interactions with MXene surface terminations to improve structural stability of the hybrid composite [55]. Despite these advantages, the application of MOFs is limited by their poor electrical conductivity and stability under aqueous conditions. The integration of MOFs with MXenes overcomes these limitations by providing electrical pathways, surface accessibility, and structural reinforcement to prevent disintegration [56]. The hierarchical porosity of MOFs on the surfaces or within the layers of MXene–MOF hybrids further promotes ion mobility, pollutant infiltration, and accelerated catalytic turnover rates for wastewater treatment.

2.2.3 | MXene–MOF Hybrids: Interfacial Bonding and Synergistic Effects

Surface compatibility is another important factor affecting the performance of MXene–MOF hybrids in wastewater treatment applications. This is because well-engineered surfaces provide excellent interfacial bonding, which improves stability, facilitates electron and ion transport, and increases the number of active sites [57, 58]. The negatively charged MXene surface enables electrostatic attraction of cations in the MOF precursors [59], followed by coordination bonding of surface groups with metal ions in MOFs to produce $Ti-O-M$ or $Ti-N-M$ bonds. Additional covalent functionalization using organic modifiers, such as silanes and dopamine, further enhances interfacial bonding while introducing additional nucleation sites for controlled MOF growth.

Furthermore, the spacing between MXene layers can suppress the uncontrolled growth of MOFs, thereby providing finer and more uniform particles with a high surface area. For example, MXene confinement decreases MOF particle size from hundreds to tens of nanometers, thereby increasing active area and efficiency of catalyst [60]. This templating mechanism promotes hierarchical or dendritic structures that facilitate mass diffusion and access to active sites. Besides, interfacial interactions govern the hybrid morphology [61], where strong MXene–MOF interactions facilitate the formation of dendritic, rod-like, or core-shell architectures with improved surface area and pore accessibility for enhanced catalytic and adsorption properties. For example, Ti_3C_2 -modulated MIL-125- NH_2 composites produced a higher H_2O_2 yield with effective degradation of organic pollutants owing to the improved interfacial design that facilitated charge separation and mass transport. Research on density functional theory has reported that electron density redistribution at the MXene–MOF interface lowers the activation energy for redox reactions, thereby enhancing electrocatalytic activity in wastewater treatment.

2.3 | Morphology and Architecture of MXene–MOF Hybrid Nanocomposites

Several structural architectures of MXene–MOF hybrids have been reported, including 2D–2D, 2D–3D, core–shell, sandwich structures, and hierarchical porous frameworks, depending on the synthesis process and interfacial chemistry. Each architecture offers specific advantages based on its functional requirements.

2.3.1 | 2D–2D Hybrids

Among the reported MXene–MOF architectures, 2D–2D hybrids provide one of the most effective platforms for interfacial synergy, given that both MXene and MOF components retain their sheet-like geometry and assemble into interleaved lamellar heterostructures with a maximized contact area. In this configuration, ultrathin MOF nanosheets nucleate directly on MXene layers to generate stacked assemblies that combine high surface exposure with minimal electron/ion transport distance, which is desirable for adsorption and electrochemistry-dominated applications. A common fabrication approach is controlled in situ growth, where

MOF nucleation occurs on the surface of MXene via coordination interactions between surface terminations ($-\text{OH}$, $-\text{O}$, $-\text{F}$) and metal precursors [62]. For example, Ni- or Co-based MOF nanosheets grown on $\text{Ti}_3\text{C}_2\text{T}_x$ can form continuous nanometer-thin coatings, while microscopy reveals ordered sheet-on-sheet structures in which MOF nanosheets act as spacers to suppress MXene restacking [63]. Functionally, these hybrids offer (i) accelerated interfacial charge transfer, where metallic MXenes compensate for the conductivity limitations of MOFs and reduce charge-transfer resistance [64], and (ii) high accessibility of active sites, as 2D MOFs expose abundant metal nodes and ligands while forming interlayer nanochannels that facilitate ion diffusion and improve reaction kinetics [65]. This characteristic is particularly important for pollutant removal and electrochemical sensing, where surface interactions control the overall behavior. In addition, the multilayer structure creates interlayer nanochannels that enhance ion diffusion and further improve reaction kinetics. Although synthesis remains challenging due to the intrinsic preference of many MOFs for 3D crystallization (e.g., requiring careful control of precursor concentration, reaction temperature, and growth duration to achieve uniform nanosheets) [66], 2D–2D MXene–MOF hybrids remain a leading architecture for maximizing interface-driven performance enhancement.

2.3.2 | 2D–3D Hybrids

2D–3D MXene–MOF hybrids have been widely reported because most MOFs crystallize into stable 3D polyhedral structures. The 3D MOF particles/crystals (e.g., ZIF-8, ZIF-67, MIL-101, UiO-family) are immobilized on conductive MXene sheets ($\text{Ti}_3\text{C}_2\text{T}_x$, Nb_2C) to form heterostructures that integrate electron transport, structural support, and porous active sites [67]. MXenes function as conductive scaffolds and nucleation substrates for uniform MOF dispersion and prevent severe particle aggregation, as observed by SEM/TEM and elemental mapping analyses. The resulting architecture enhances performance by coupling MOF-derived hierarchical porosity and high-density active sites with MXene-enabled rapid electron transfer, thereby reducing kinetic and resistive limitations [68]. This synergy is particularly important for electrocatalysis (e.g., OER/HER), where fast reactant access, efficient charge transport, and rapid product release affect activity and stability of reaction [28]. Nevertheless, excessive MOF loading can hinder MXene conduction pathways and affect electrical connectivity, highlighting the importance of optimizing the MOF size, surface coverage, and spatial distribution to maximize interfacial interactions [69]. Ultimately, 2D–3D hybrids present a scalable and adaptable approach to co-engineer conductivity, porosity, and catalytic functionality, making them suitable for applications in environmental remediation and wastewater treatment.

2.3.3 | Core–Shell and Sandwich-Type Structures

Core–shell and sandwich-type MXene–MOF architectures represent advanced interface-engineering strategies that directly address the key bottlenecks that limit the practical use of such materials, such as oxidation susceptibility, structural instability, and inefficient active-site utilization in aqueous systems. In core–shell designs, conformal encapsulation allows deliberate

functional partitioning, where MXene-core/MOF-shell structures protect MXenes from oxidation while simultaneously introducing porous adsorption/catalytic domains, with tunable shell thickness to balance interfacial protection and mass-transfer kinetics [70]. Conversely, MOF-core/MXene-shell hybrids leverage MXenes as conductive and mechanically compliant coatings to enhance electrical connectivity and buffer volumetric stress, thereby improving the durability and cycling stability of MOF-derived active phases. Sandwich-type assemblies further intensify synergistic coupling by constructing ordered multilayers in which MOFs act as interlayer “pillars” to prevent MXene restacking and preserve continuous ion-transport pathways. Notably, advanced probes (e.g., STEM/XAS) suggest that such architectures can stabilize highly active interfacial metal motifs, including atomically dispersed sites. Consistent with this structure–function rationale, Figure 6 demonstrates that layered MXene–MOF hybrids maintain a sustained electrochemical output after prolonged operation, indicating robust interfacial integration and minimization of active-phase detachment. The significantly increased C_{dl} relative to pristine components further confirms an expanded electrochemically accessible surface, reflecting the formation of a hierarchical porous network coupled to a continuous conductive scaffold [48]. Overall, core–shell and sandwich MXene–MOF topologies offer a powerful route to simultaneously optimize stability, transport, and active-site efficiency, making them highly promising for water-based catalysis and environmental remediation, where long-term operational robustness is mandatory.

2.3.4 | Hierarchical Porous Frameworks

Hierarchical porous MXene–MOF hybrids can be considered an advanced structural design because they incorporate multi-length-scale porosity to address diffusion bottlenecks associated with microporous MOFs. These frameworks combine MOF-derived micropores, interparticle mesopores, and macroporous channels from MXene aerogels or 3D scaffolds to create interconnected networks that improve accessibility, transport kinetics, and active-site utilization [71]. In addition, MXenes serve as conductive scaffolds that preserve electrical percolation and mitigate pore collapse during post-treatment, while MOFs or their derived porous carbons and metal compounds introduce a high density of catalytically active sites. The resulting hierarchical architecture integrates macropores that facilitate bulk diffusion, mesopores that accelerate ion and solute transport, and micropores that provide abundant adsorption and reaction sites, thereby improving mass-transfer kinetics across multiple length scales [72]. Despite these advantages, multistep fabrication procedures and the sensitivity of pore formation to synthesis conditions limit reproducibility and scalable production, which necessitates more robust and controllable synthesis strategies [73]. Hierarchical porous systems thus enable the synergistic integration of conductivity, tunable porosity, and mechanical stability within a unified framework.

3 | Mechanisms in Wastewater Treatment

The integration of MXenes with MOFs produces hierarchical hybrid materials that combine a high surface area, tunable

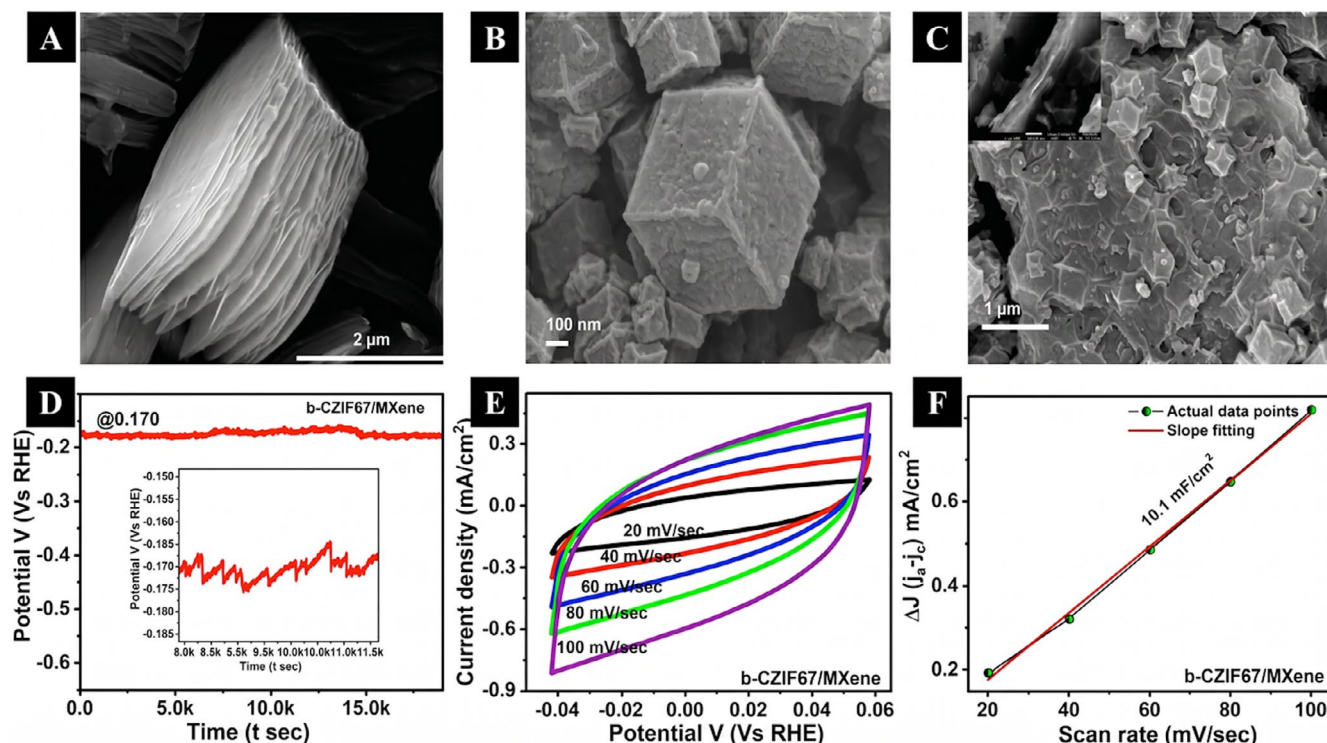


FIGURE 6 | SEM images of (A) MXene sheet, (B) bi-ligand ZIF-67, and (C) MXene-MOF composite. (D) Chronopotentiometric stability of MXene-MOF under constant current (E) Cyclic voltammetry in non-Faradaic region at varying scan rates for MXene, MOF, and MXene-MOF composite indicating increased surface accessibility. (F) Capacitive current against scan rate for double layer capacitance (C_{dl}) determination, which shows the large active surface area arising from hierarchical porosity of MXene-MOF structure. Reproduced from [48] with permission from Wiley Publications.

porosity, redox-active sites, and electrically conductive pathways for multimodal pollutant removal in complex water bodies. MXene-MOF hybrids provide physicochemical platforms for mass transfer, surface reactivity, and charge transport to occur simultaneously in wastewater treatment to target various pollutants, such as heavy metals, dyes, pharmaceuticals, and other emerging organic pollutants. Wastewater treatment using MXene-MOF hybrids is governed by four interrelated mechanisms: adsorption, photocatalysis, membrane separation, and electrochemical transformation. First, adsorption is a surface phenomenon that uses the surface chemistry and pore structure of the hybrid material for the rapid capture of pollutants from wastewater. Second, the photocatalysis process uses interfacial charge separation to produce reactive species for the oxidative degradation of pollutants in wastewater. The membrane separation process uses controlled transport pathways for size- and charge-selective filtration of pollutants, whereas electrochemical processes allow redox-driven conversion and regeneration of pollutants. It should be noted that the aforementioned mechanisms can occur concurrently, as interfacial coupling between the conductive MXene phase and catalytically active MOF domains promotes synergistic behavior, which enhances reaction rates, minimizes fouling, and extends the operational lifetimes of the electrodes. Concurrent membrane separation, photocatalytic degradation, electrochemical processes, and adsorption mechanisms for effective pollutant removal from wastewater are shown in Figure 7A–D, respectively. Table 2 presents a summary of the literature findings regarding MXene-MOF hybrids used in wastewater treatment. It includes information on the

target pollutant, the mechanism of pollutant removal, and the main findings reported. This overview aims to offer a mechanistic insight that can guide the rational design of materials and enhance performance in future water remediation technologies.

3.1 | Membrane Separation Mechanisms

Membrane-based separation is an essential process in modern wastewater treatment for continuous operation, scalability, and integration with existing filtration systems [93]. For example, the MXene-BIC@MIL-101(Fe) hybrid membrane exhibited photocatalytic self-cleaning properties that enabled the composite to maintain a flux recovery ratio of $\geq 90\%$ after multiple filtration cycles [92].

MXene-based membranes combine the strengths of conventional size-exclusion and adsorptive membranes, providing precise size-based separation together with strong adsorption owing to their unique surface chemistry. However, MXene sheets tend to restack and aggregate due to van der Waals interactions, and they can swell in aqueous environments, which reduces their filtration performance [94]. MOFs offer several advantages over traditional adsorbents and catalysts: (i) their pore sizes and surface properties can be easily adjusted, affording high specificity; (ii) isoreticular MOFs can be synthesized from the same metal by simply changing the ligand length; (iii) many metal cations can form MOFs, whereas only a few (Si, Al, P) can form other adsorbents; (iv) zeolite-type materials require inorganic or organic

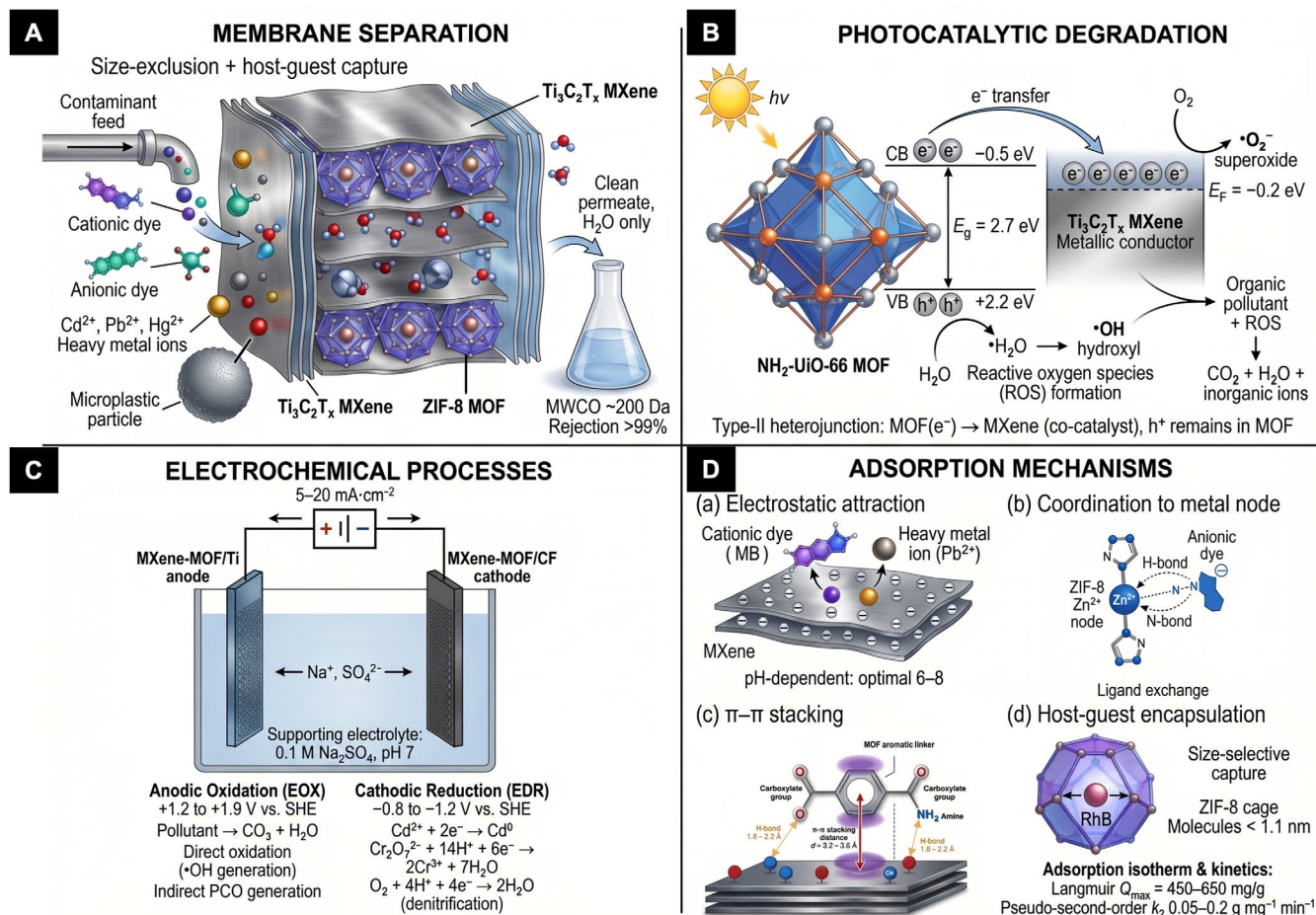


FIGURE 7 | Key mechanisms of MXene–MOF hybrids in wastewater treatment (A) membrane separation (B) photocatalytic degradation (C) electrochemical processes and (D) adsorption.

templates, but MOFs can use the solvent itself as a template; and (v) different metal components can be incorporated into MOFs using the same ligands or their analogs [95].

For example, a poly(vinylidene fluoride) (PVDF) membrane modified with UiO-66-NH₂ (denoted U5P1) exhibited improved hydrophilicity and porosity. The water contact angle decreased from 68.4° to 25.4°, while the underwater oil contact angle increased from 139.5° to 150.5°, resulting in a surface that was simultaneously superhydrophilic and underwater oleophobic. The membrane demonstrated outstanding separation performance, achieving > 99% oil removal from emulsions and > 99% rejection of Congo red dye, with a high permeation flux of 1520 L m⁻² h⁻¹. Additionally, the membrane sustained > 95% rejection and achieved flux recovery ratios exceeding 81% over multiple cycles, demonstrating excellent antifouling performance and operational stability [96]. These findings highlight the potential of MOF-modified membranes for efficient and durable water treatment applications.

3.2 | Photocatalytic Mechanisms

Photocatalytic degradation is a widely employed advanced oxidation process (AOP) used for the mineralization of recalcitrant organic pollutants such as dyes, pharmaceuticals, and pesticides

[97]. Ti₃C₂T_x MXene has emerged as an attractive component in hybrid photocatalysts owing to its metallic conductivity, hydrophilic surface chemistry, strong adsorption affinity, and ability to promote rapid interfacial charge transfer [98].

MOFs incorporating photoactive metal centers, such as Fe, Ti, or Co, can absorb photons and generate electron–hole pairs (EHPs). However, pristine MOF materials suffer from limited structural stability and low EHP separation efficiency, which markedly constrain their performance in photocatalytic H₂ production. To overcome these drawbacks, MOF-based hybrids composed of MOFs integrated with one or more functional materials combine the inherent advantages of MOFs (rich catalytic active sites, diverse pore structures and large SSA) with the unique optical, electrical, magnetic, and catalytic properties of the added components, thereby endowing the hybrids with enhanced physicochemical characteristics that markedly improve photocatalytic efficiency [99, 100]. The introduction of MXenes addresses this limitation because the metallic conductivity and high carrier density of MXenes act as electron sinks [101] to promote rapid electron transfer from the photoexcited MOF conduction band to the MXene surface [102]. This interfacial charge transfer does not only suppress recombination but also enhances the generation of reactive oxygen species (ROS), such as hydroxyl (•OH) and superoxide (•O₂⁻) radicals, which are primarily responsible for oxidative degradation of pollutants

TABLE 2 | MXene–MOF hybrid systems for wastewater treatment: Target pollutants, mechanisms and key performance outcomes.

Target pollutant/ Category	Representative MXene–MOF hybrid	Treatment mechanism	Key performance/Outcome	References
Heavy metals (Pb ²⁺ , Cu ²⁺)	V ₂ C MXene@ZIF-8	• Pb–π interaction • Pb–complexation with MXene oxygenated groups • Electrostatic attraction; pore filling • Interaction with Zn sites in ZIF-8, strong binding energy (–2.15eV)	• High Pb(II) adsorption capacity (370.4 mg g^{–1}) • 94% removal efficiency (84.2% after five cycles) • Selective removal in binary solution (87% Pb²⁺ vs. 62% Cu²⁺)	[74]
Heavy metals/ Radioactive metals (U(VI))	Carbonized MIP-202/ MXene (CMM)	• Electrosorption in capacitive deionization • Enhanced conductivity, pore structure, and nitrogen sites • Prevents MXene aggregation	• Maximum adsorption capacity 582.46 mg g^{–1} • Removal ratio 89.1% at 1.2 V; high selectivity for UO₂²⁺ (92.3%) in multi-ionic solution • Improved charge transfer and mechanical robustness	[75]
Uranium (U(VI))	UiO-66-NH ₂ / MXene aerogel	• Adsorption via mesoporous structure, surface complexation, and electrostatic interaction • Suitable for capacitive deionization	• Maximum adsorption capacity 229.1 mg g^{–1} • > 96% removal efficiency after five adsorption–desorption cycles • Easy separation and structural stability	[76]
Heavy metals (Cr(VI))	MXene@MIL-53-NH ₂	• Adsorption and simultaneous reduction of Cr(VI) to Cr(III) • Enhanced electron transfer via MXene • Strong binding to oxyanions	• High adsorption capacity (224.46 mg g^{–1}) • High removal at pH3 • Good recyclability and ionic interference resistance	[77]
Heavy metals/ Organic dyes (Cr(VI), Tetracycline, TC)	Alkalized MXene/ Co-MOF (alk-MXene/ Co-MOF)	• Adsorption via electrostatic interaction, hydrogen bonding, and π–π stacking • Nanochannel formation enhances water permeability	• High water permeability (443.7 L m^{–2} h^{–1} bar^{–1}) • > 98% removal for Cr(VI) and TC • High breakthrough/saturation volumes (up to 4900 mL for Cr(VI), 6400 mL for TC) • Maintains > 95% removal after 10 cycles; preferential TC separation confirmed by DFT	[78]
Organic pollutants (dyes and antibiotics): Methyl orange (MO), Ciprofloxacin (CIP)	Ti ₃ C ₂ T _x @ZIF-8 (MX@ZIF), MXO@ ZIF, MXOH@ZIF	• Enhanced electrostatic interactions and hydrogen bonding from –O and –OH terminal groups • Dominant van der Waals interactions; non-covalent interactions • Increased pollutant–substrate contact frequency for stronger adsorption	• Strong adsorption of MO and CIP • High van der Waals energies (–253.454 kJ/mol for MXOH@ZIF–CIP) • –201.660 kJ/mol for MXOH@ZIF–MO) • MXOH@ZIF shows highest pollutant affinity; validated by MD simulations and AIM calculations	[40]

(Continues)

TABLE 2 | (Continued)

Target pollutant/ Category	Representative MXene–MOF hybrid	Treatment mechanism	Key performance/Outcome	References
Organic contaminants (antibiotics): Ciprofloxacin (CIP)	VCo-MOF@Ti ₃ C ₂ T _x composite catalyst	• Peroxymonosulfate (PMS) activation via synergistic transition-metal active centers (V–Co–Ti) • Multiple degradation pathways including electron-transfer processes • Enhanced PMS adsorption and activation (DFT-validated) • Formation of superoxide radical species due to catalyst hydrophilicity • Rich active sites promoting catalytic oxidation	• 96.14% CIP removal (20 mg/L) within 30 min using only 5 mg catalyst • Effective in different real-water environments • Electrochemical tests (CV, LSV) demonstrate electron-transfer pathway • Strong PMS activation ability predicted by DFT	[79]
Organic pollutants/ Antibiotics (Tetracycline, TTCH)	2D MOF-derived carbon/Fe ₃ O ₄ (NSC@Fe ₃ O ₄)	• Heterogeneous Fenton-like catalytic degradation via non-radical pathways (¹O₂ and electron transfer) • Size-exclusion effect of 2D layers	• Effective TTCH removal under coexistence with humic acid • Selective degradation confirmed • Reduced toxicity of intermediates	[80]
Organic pollutants/ Antibiotics and dyes (Tetracycline, Rhodamine B) and Pathogens (MRSA, <i>E. coli</i>)	Porphyrinic MOF (PCN-224)/ Ti ₃ C ₂ -MXene	• Photo-thermal-enzyme synergistic degradation via Schottky junction for enhanced charge separation photothermal effect, and peroxidase-like catalytic activity	• 91.2% tetracycline and 97.4% Rhodamine B degradation within 60 min • 99.99% MRSA and 99.92% <i>E. coli</i> inactivation • Multimechanistic, scalable approach	[81]
Emerging organic pollutants (PFAS: PFOA, PFHpA, PFHxA)	Iron-based MOF/ polydopamine-coated MXene (DMMIL/PD@ Ti ₃ C ₂ T _x) in cellulose acetate mixed- matrix membrane	• Adsorption and size-exclusion via MOF pores • Enhanced water transport through MXene • Synergistic nanofiller-membrane interaction	• Enhanced water flux (1.42×) • Improved PFOA rejection (1.65×) vs. pristine CA • Removal from real wastewater: 60% PFOA, 57% PFHpA, 55% PFHxA • Maintained 54%–68% flux recovery after 5 cycles	[82]
Emerging organic pollutants/Disinfection byproducts (IAN, BAN, CAN)	TiNbC/MnCO ₃ @ MOF incorporated into sodium alginate hydrogel (TiNbC/ MnCO ₃ @MOF-SA)	• Adsorption via hydrogen bonding and pore-facilitated uptake • High surface area and mesoporosity enhance interaction with DBPs	• High adsorption capacity: 648 mg g⁻¹ (IAN), 642 mg/g (BAN), 632 mg g⁻¹ (CAN) • Optimal at pH 6–7; excellent reusability up to 15 cycles	[83]

(Continues)

TABLE 2 | (Continued)

Target pollutant/ Category	Representative MXene–MOF hybrid	Treatment mechanism	Key performance/Outcome	References
Antibiotics/Salt separation	ZnBDC-NH ₂ MOF/ MXene membrane	- Electrostatic assembly - Size-exclusion - Hydrogen bonding - Fast water transport via MXene nanochannels	97.59% chloramphenicol rejection - Water permeance 269.3 L m⁻² h⁻¹ bar⁻¹ - Stable for 120 h - High antibiotic/salt selectivity - Performance superior to most reported membranes	[7]
Metalloids/Toxic oxyanions (As(III) and As(V))	Fe–ZIF-8@MXene	- Van der Waals interactions; surface adsorption - Chemical complexation; electrostatic interactions - Formation of multiple surface complexes from functional groups on MXene and Fe-doped ZIF-8	- High BET surface area (531.7 m² g⁻¹) - Langmuir isotherm behavior ($R^2 = 0.998$ for As(III), 0.997 for As(V)) - High removal efficiency in real water samples (91.07% for As(III), 98.96% for As(V)) - Stable structural integrity after adsorption	[84]
Synthetic dyes: Methylene blue (MB), Acid blue 80 (AB)	MXene, MOF (used separately as adsorbents)	- Electrostatic interactions (cationic MB with MXene, anionic AB with MOF) - Hydrophobic interactions (MOF capturing MB) - Adsorption influenced by pH, ionic strength, and co-existing ions - Rapid kinetics and selective adsorption	- MXene: fast adsorption kinetics, selective for MB, surface area 9 m² g⁻¹ - MOF: high adsorption capacity (~200 mg g⁻¹ for AB, ~140 mg g⁻¹ for MB), surface area 630 m² g⁻¹ - Effective under various solution conditions - Economical for wastewater treatment	[85]
Organic dye: Methylene blue (MB)	Fe-free dual MOF nanoparticles: HKUST-1/ZIF-67-X (core–satellite architecture)	- Fenton-like catalytic degradation via H₂O₂ activation - Synergistic effect between HKUST-1 and ZIF-6 - No Fe ions involved → avoids sludge formation	- High catalytic activity: 93.29% MB degradation in 40 min - Retains 80.17% efficiency after five cycles - Cost-effective, environmentally benign, reusable - Effective under near-neutral pH	[86]
Organic dyes (methyl orange, MO; direct red 31, DR31)	3D-printed Ti ₃ C ₂ T _x MXene/UfO-66 architectures (grid, star, honeycomb geometries)	- Adsorption via high surface area and hierarchical porous structures - Immobilization of MXene/UfO-66 within 3D-printed lattices to avoid secondary pollution - Dye capture facilitated by electrostatic and surface interactions	- Specific surface area: 347.28 m₂/g, pore volume: 0.26 cm³/g - Dye removal efficiency: MO 88.95%, DR31 76.98% (honeycomb geometry) - Good reusability: stable performance after four cycles	[3]
Organic dyes (Methylene Blue, MB)	Ni-MOF/MXene (NM@MX)	Adsorption via electrostatic interactions, π–π stacking, and hydrogen bonding	- High adsorption capacity (1012.37 mg g⁻¹) - Mesoporous structure (~31 nm); kinetics described by fractional model ($R^2 = 0.9968$)	[6]

(Continues)

TABLE 2 | (Continued)

Target pollutant/ Category	Representative MXene–MOF hybrid	Treatment mechanism	Key performance/Outcome	References
Organic dyes (Methylene Blue, MB)	Ti ₃ C ₂ Tx MXene (ultrasonication-assisted, US-MXene)	• Adsorption via electrostatic interactions • Improved dispersion and oxygenated functional groups via ultrasonication	• High selectivity for MB • Fast adsorption kinetics • Effective under various water chemistry conditions • High regeneration after four adsorption–desorption cycles	[87]
Organic dyes (Rhodamine B, Congo Red, Methyl Orange)	Ti ₃ C ₂ Tx MXene/ZIF-8 MOF, modified with tannic acid and polyphenols (Ti ₃ C ₂ T _x @ZIF-8@TA)	• Photocatalytic degradation under visible light • Enhanced heterogeneous interfaces and cross-linked network • Improved charge separation and light absorption	• High degradation efficiency: ~87% RhB, 85% Congo Red, 79% Methyl Orange within 60 min • Low energy consumption, environmentally compatible, non-toxic, and cost-effective	[88]
Antiviral drug/organic contaminant: Ribavirin (RBV)	Carboxyl-functionalized MXene with NH ₂ [−] UiO-66 (molecularly imprinted MOF) → CXPM-MIMs	• Molecularly imprinted adsorption for selective recognition • Carboxylate-assisted coordination creates strong linkage between MXene and MOF • Selective adsorption via imprinting sites • Heterostructure facilitates specific binding and separation	• High adsorption capacity: 58.3 mg g^{−1} • Strong permselectivity for RBV ($\beta = 4.89\text{--}10.14$) • Excellent molecular recognition in multi-component solutions • In situ MOF growth ensures stable heterostructure	[89]
Salt/desalination: NaCl (3.5 wt % solution)	Ti ₃ C ₂ T _x MXene@MOF-303	Composite membrane adsorption/separation • MXene provides functional groups and layered structure, MOF-303 contributes porosity • Blended into PVA/PAN membrane for pervaporation-based desalination	• High pervaporation flux: 15.87 kg·m^{−2}·h^{−1} High salt rejection: 99.84% at 35°C • Enhanced separation performance due to synergistic MXene–MOF structure	[90]
Cationic and anionic dyes, salts (Na ₂ SO ₄ , MgSO ₄ , MgCl ₂ , NaCl)	UiO-66-NH ₂ @MXene 2D nanocomposite (modified PES membrane)	Membrane-based adsorption/separation • MXene provides functional groups and layered structure • UiO-66-N₂ adds porosity and hydrophilicity • Synergistic effect enhances water flux, dye/salt rejection, and anti-fouling properties	• Dye removal: 72%–81% for cationic dyes, > 91% for anionic dyes • Salt rejection: 62%–91% depending on salt • Water flux: > 4× increase • Water contact angle decreased from 65° to 38° • Improved anti-fouling performance	[47]
Anionic dyes (methyl orange, direct red 31)	3D-printed lattice decorated with MXene/MOF hybrid (3D-MXOF)	Adsorption via • High surface area and porosity of MXOF • Synergistic interactions between MXene functional groups and MOF • Facilitated adsorption on a hierarchical 3D lattice for enhanced accessibility	• High dye removal: 91.98% (methyl orange), 84.9% (direct red 31) • Fast adsorption kinetics (pseudo-first-order model) • Recyclable: stable performance after four adsorption–desorption cycles	[35]

(Continues)

TABLE 2 | (Continued)

Target pollutant/ Category	Representative MXene–MOF hybrid	Treatment mechanism	Key performance/Outcome	References
Oil-in-water emulsions, high-viscosity crude oil	PEG/MXene@UiO- 66-NH ₂ membrane (intercalation-induced lamellar structure)	Membrane-based separation • MOF nanoparticles intercalate MXene nanosheets to stabilize interlayer spacing • PEG enhances hydrophilicity and hydrogen bonding, improving swelling resistance • Increased lamellar roughness and water retention enhance selectivity and fouling resistance	• High permeability: 1246 ± 12 L·m ⁻² ·h ⁻¹ ·bar ⁻¹ • Oil removal efficiency: > 99.7% • Stable layer expansion: 0.05 nm after 8 days in water • Superior antifouling: UWOSA > 156°, UWOSA < 5.5° • Excellent chemical durability and mechanical robustness (corrosive environments, high-salt, ultrasonic, bending, abrasion tests)	[91]
Oily wastewater (oil-in- water emulsions)	MXene-MOF composite membrane with BIC@MIL-101(Fe) nanoparticles	• Membrane separation with hydrophilic modification • Photocatalytic self-cleaning via BIC@ MIL-101(Fe) • Anti-fouling through reduced oil adhesion and XDLVO-guided surface interactions	• High water flux: 2534.89 ± 13.63 L·m ⁻² ·h ⁻¹ ·bar ⁻¹ • Separation efficiency > 99.7% • Superhydrophilicity: water contact angle < 5° in 5 s • Excellent recyclability: flux recovery rate ≥ 90% after 10 cleaning cycles	[92]

into harmless products [103]. MXene/MOF composite materials have therefore shown strong potential for pollutant degradation, owing to their distinctive physicochemical characteristics and synergistic interfacial effects. In these hybrids, [104]. MXene with superior electrical conductivity acts as an electron mediator to facilitate the transfer of photoexcited electrons from the MOF to the MXene surface. The interfacial interaction allows for an efficient charge transport pathway, which enhances charge separation and suppresses electron-hole recombination; thus, improving photocatalytic efficiency.

The band alignment and interfacial contact area between the MOF and MXene determine the efficiency of the photocatalytic process [105]. Optimized hybrids, such as ZIF-8, Ti₃C₂T_x@TA, Ti₃C₂T_x/ZIF-8@TA10, Ti₃C₂T_x/ZIF-8@TA20, and Ti₃C₂T_x/ZIF-8@TA30 photocatalysts, have demonstrated excellent performance under visible-light irradiation, achieving degradation efficiencies of approximately 87%, 85%, and 79% for RhB, Congo red, and methyl orange, respectively, within 60 min [88]. These hybrids also exhibit enhanced durability, similar to that observed in Ti₃C₂/NiCo-MOF composites fabricated via vacuum-based filtration, where robust hydrogen bonds between Ti₃C₂ and NiCo-MOF further strengthen the structural durability, thereby providing practical advantages for their integration into photocatalytic reactors and solar-assisted wastewater treatment systems [106].

3.3 | Electrochemical Treatment Mechanisms

Electrochemical treatment using MXene–MOF hybrids is governed by controlled interfacial reaction kinetics and the in situ generation of reactive species that facilitate both pollutant degradation and metal ion recovery. Within this architecture, MXene serves as a highly conductive scaffold that establishes continuous electron-transport pathways across the electrode interface [107], whereas the MOF component contributes abundant redox-active coordination centers, such as Fe²⁺/Fe³⁺ and Co²⁺/Co³⁺ couples, that mediate oxidation–reduction reactions [108]. The negatively charged surface terminations of MXene enhance electrostatic interactions with cationic contaminants [109], while the intrinsic porosity and functional diversity of MOFs introduce additional adsorption domains. This cooperative interaction promotes efficient electrosorption under an applied potential, enabling the removal of heavy metal ions including Ni²⁺, Cd²⁺, Cu²⁺, and Zn²⁺ [110].

Additionally, MXene–MOF hybrids function as effective electrocatalysts in electro-Fenton systems, where the electrochemical reduction of dissolved oxygen generates reactive oxygen species that can oxidize organic contaminants into less toxic intermediates [107]. The porous framework of the MOF facilitates mass transport of reactants and intermediates [111], while the high electrical conductivity of MXene accelerates electron transfer processes that are essential for radical generation [112]. These structural and electronic characteristics also underpin their performance in capacitive deionization applications, where the combination of MXene’s two-dimensional conductive layers and the hierarchical porosity of MOFs enables high ion storage capacity and rapid, reversible adsorption–desorption cycles with reduced energy demand [113]. Furthermore, the hybrid interface

increases the density of accessible active sites for electrocatalytic reactions, where MXene provides electron-rich surfaces that promote rapid charge transfer, whereas MOFs offer tunable coordination environments that support selective adsorption and catalytic transformation.

In wastewater treatment systems, electrochemical processes operate in concert with adsorption, photocatalysis, and membrane-based separation. Adsorption concentrates pollutants proximal to catalytic sites, thereby enhancing degradation kinetics, while membrane selectivity governs size- and charge-dependent separation without limiting accessibility to reactive interfaces. Continuous regeneration of electroactive sites sustains adsorption capacity during operation, and the integration of these mechanisms results in enhanced removal efficiency with mitigated fouling effects.

3.4 | Adsorption Mechanisms

Adsorption is the most fundamental and widely used mechanism in wastewater treatment, particularly for the removal of heavy metals, synthetic dyes, and organic micropollutants [114]. In MXene–MOF hybrid systems, adsorption arises from a combination of surface complexation, electrostatic attraction, ion exchange, coordination bonding, and π – π stacking interactions [115].

The 2D layered structure of MXenes (e.g., $\text{Ti}_3\text{C}_2\text{T}_x$, Nb_2CT_x , and V_2CT_x) provides a large accessible surface area with abundant surface terminations ($-\text{O}$, $-\text{OH}$, $-\text{F}$, and $-\text{Cl}$), which act as active binding sites for cationic and anionic species. In contrast, the porous MOF component introduces high surface area and adjustable pore chemistry that enhances mass transport and facilitates selective adsorption [116–119]. The interfacial coupling between MXenes and MOFs enhances the adsorption performance of the composite by ensuring a uniform distribution of active sites, improving structural stability, and facilitating rapid pollutant transfer [6]. This synergistic integration minimizes aggregation and diffusion resistance, thereby overcoming two major drawbacks of single-component adsorbents.

Hybridization effectively enhances intraparticle diffusion rates and reduces external mass-transfer resistance, leading to shorter equilibration times and higher adsorption capacities. For instance, MXene@MOF hybrids, such as Fe_3O_4 @MXene@MOF-74, have demonstrated high adsorption capacities for the fungicides epoxiconazole and tebuconazole, reaching 120.96 and 108.26 mg g^{-1} , respectively [120]. The UiO-66/MXene (derived from Ti_3AlC_2) composite exhibited excellent adsorption performance, with dye and antibiotic removal efficiencies of 97%–99% [121]. The combination of MOF and MXene led to an increased distribution coefficient ($L_g K_d = 4.8$), indicating a strong binding affinity for Cr(VI) oxyanions and improved Cr(VI) adsorption in MXene@MIL-53- NH_2 , with a theoretical adsorption capacity of 224.46 mg g^{-1} [77]. Additionally, 3.3% MXene/Cu-MOF demonstrated superior adsorption performance for methyl phenyl sulfide in model fuel, achieving an equilibrium adsorption capacity of 87.4 mg g^{-1} [122]. Furthermore, these hybrids exhibited remarkable reusability

over multiple cycles with minimal capacity loss. For instance, 3D-printed MXene/UiO-66 structures maintained good reusability and stability after four cycles [3], and the 3D amidoxime-functionalized $\text{Ti}_3\text{C}_2\text{T}_x$ /ZIF-67 structure retained a reusability rate of 63.51% after 10 cycles [123], highlighting their potential for use in continuous flow or column-type adsorption systems.

However, a direct comparison across studies is challenging because the values reported for maximum adsorption capacities can vary based on the initial pollutant concentration, experimental conditions and testing standards. For example, negatively charged MXene surfaces in neutral to alkaline conditions have shown higher adsorption capacities that is, $>1000 \text{ mg g}^{-1}$ toward MB dye due to the planar aromatic structure, strong π – π interactions, and enhanced electrostatic attraction [6]. In contrast, fungicides and other structurally complex organic molecules have reported lower adsorption capacities of $\sim 100 \text{ mg g}^{-1}$ because of their larger molecular size, steric hindrance, lower charge density, and poor interaction with surface functional groups, which limits diffusion into pores [124].

The adsorption capacity is also affected by pH and ionic strength. At low pH, protonation of MXene surface terminations ($-\text{OH}$ to $-\text{OH}_2^+$) and MOF functional groups reduces electrostatic attraction toward cationic pollutants while favoring the adsorption of anionic species through electrostatic interactions [125, 126]. In contrast, under alkaline conditions, deprotonation of surface groups enhances the negative surface charge to promote the adsorption of cationic contaminants via electrostatic attraction and surface complexation. It should also be noted that surface complexation and coordination bonding are desirable for heavy metal ions such as Pb^{2+} and Cr(VI) due to strong interactions with oxygen-containing functional groups on MXene and metal nodes in MOFs, while π – π interactions and hydrophobic effects are prominent for aromatic organic pollutants such as dyes and pharmaceuticals [127].

Besides, high ionic strength compresses the electrical double layer on MXene surfaces, thereby weakening long-range electrostatic attraction and shifting the dominant mechanism toward inner-sphere complexation or pore-filling effects [128, 129]. Moreover, competitive adsorption is likely to occur when ions of similar charge are present, such as in multicomponent systems, which can reduce adsorptive performance. In these systems, selectivity does not depend on electrostatic interactions but rather on pore size distribution, presence of functional groups, and metal–ligand affinity [130]. In addition, the structure of MXene–MOF hybrids affects the condition-dependent performance of the aforementioned hybrids. For instance, MXenes with higher densities of $-\text{O}$ and $-\text{OH}$ terminations exhibit stronger metal-binding affinity through surface complexation, while MOFs with smaller pore structures promote size-selective adsorption with better mass transfer, although with limited diffusion rates [129]. Hence, adsorption performance depends on various factors, such as interfacial chemistry, pore structure, and surrounding conditions, all of which determine the main pollutant removal mechanism.

4 | Applications in Wastewater Treatment

4.1 | Heavy Metal Removal

MXene–MOF hybrids are highly effective sorbents for the removal of toxic heavy metals via multiple pathways, including electrostatic attraction, surface complexation, ion exchange, and redox reactions. For example, V_2C MXene@ZIF-8 demonstrated a strong affinity toward Pb^{2+} through synergistic $Pb-\pi$ interactions, coordination with MXene oxygen-containing functional groups, electrostatic adsorption, pore-filling effects, and Zn-site binding within the ZIF-8 framework. The hybrid achieved a maximum adsorption capacity of 370.4 mg g^{-1} and a removal efficiency of 94%, while retaining 84.2% of its initial efficiency after five adsorption–desorption cycles, confirming its reusability. Similarly, MXene@MIL-53- NH_2 effectively removed Cr(VI) through simultaneous adsorption and reduction to the less toxic Cr(III), with a maximum capacity of 224.46 mg g^{-1} , pseudo-second-order kinetics, and high recyclability under acidic conditions [74, 77].

Carbonized MIP-202/MXene composites (CMM) and UiO-66- NH_2 /MXene aerogels are effective for U(VI) removal in radioactive metal remediation. The CMM exhibits a maximum adsorption capacity of 582.46 mg g^{-1} and high selectivity for UO_2^{2+} (92.3%) in multi-ionic solutions via electrosorption, while UiO-66- NH_2 /MXene aerogels achieve >96% removal over five cycles, facilitated by mesoporous structures and capacitive deionization (CDI) mechanisms [75, 76]. Furthermore, Fe–ZIF-8@MXene demonstrated high removal efficiencies for arsenic metalloids, particularly As(III) and As(V), achieving rates of 91.07% and 98.96%, respectively (Figure 8A). This performance can be attributed to several factors, including synergistic surface adsorption, van der Waals interactions, strong chemical complexation, excellent stability and regenerability of the material [84].

4.2 | Organic Pollutant Degradation

MXene–MOF hybrids have also been reported to be effective for the removal of organic pollutants, such as dyes, antibiotics, and antiviral pharmaceuticals, via photocatalysis, adsorption, and advanced catalytic oxidation. For instance, $Ti_3C_2T_x$ @ZIF-8 composites modified with tannic acid (TA) and polyphenols achieved degradation efficiencies of 87%, 85%, and 79% for rhodamine B, Congo red, and methyl orange, respectively, within 60 min under visible-light photocatalysis, with heterogeneous interfaces promoting effective charge separation [88]. Furthermore, VCo-MOF@ $Ti_3C_2T_x$ activated peroxy-monosulfate (PMS) via synergistic metal centers for antibiotic degradation, where 96.14% of ciprofloxacin was removed within 30 min through electron-transfer pathways [79]. The composites of Porphyrinic MOF (PCN-224) combined with Ti_3C_2 -MXene enhanced photo-thermal-enzyme activity, resulting in the degradation of 91.2% of tetracycline and 97.4% of Rhodamine B, as well as the inactivation of over 99% of pathogens [81]. Additionally, heterogeneous Fenton-like degradation using 2D MOF-derived carbon/ Fe_3O_4 selectively removed tetracycline from complex water matrices (Figure 8B) [80].

Toxicity analysis based on degradation intermediates and *E. coli* culture showed that tetracycline toxicity was reduced in the NSC@ Fe_3O_4 /PMS system.

4.3 | Emerging Contaminant Removal

The integration of MXenes with MOFs yields synergistic hybrid structures for the efficient removal of emerging contaminants, such as per- and polyfluoroalkyl substances (PFAS), disinfection by-products (DBPs), and antiviral pharmaceuticals. Iron-based MOF/polydopamine-coated MXene in mixed-matrix membranes exhibited enhanced water flux and PFAS rejection (~60% PFOA removal) due to synergistic adsorption and size-exclusion mechanisms [82]. TiNbC/MnCO₃@MOF hydrogels exhibited high adsorption capacities for IAN, BAN, and CAN ($632\text{--}648\text{ mg g}^{-1}$) through hydrogen bonding and mesoporous uptake, with excellent reusability over 15 cycles [83]. Carboxyl-functionalized MXene with NH_2 -UiO-66 (CXPM-MIMs) enabled selective adsorption of ribavirin via molecular imprinting to achieve a capacity of 58.3 mg g^{-1} and strong permselectivity in multi-component solutions (Figure 8C) [89]. Furthermore, the regeneration efficiency of the CXPM-MIMs was 88.91% after 10 adsorption–desorption cycles, indicating excellent regeneration stability and separation performance after repeated cycles.

4.4 | Microplastics and Macromolecular Pollutants

MXene–MOF composites facilitate size-selective and membrane-based separation of high-molecular-weight contaminants. For oil-in-water emulsions, PEG/MXene@UiO-66- NH_2 membranes achieved >99.7% oil removal with high permeability ($1246\text{ L m}^{-2}\text{ h}^{-1}\text{ bar}^{-1}$) and excellent antifouling performance, maintained under harsh chemical and mechanical conditions (Figure 8D) [91]. Similarly, MXene–MOF composite membranes incorporating BIC@MIL-101(Fe) nanoparticles combine hydrophilicity, photocatalytic self-cleaning, and superhydrophilic surfaces to achieve >99.7% separation efficiency with rapid flux recovery (>90% after 10 cycles) [92].

4.5 | Multifunctional and Coupled Systems

MXene–MOF hybrids enable multifunctional water treatment by integrating adsorption, catalysis, and separation in a single platform. Membranes such as $Ti_3C_2T_x$ @MOF-303 and UiO-66- NH_2 @MXene-modified PES demonstrate combined desalination, dye removal, and anti-fouling capabilities. $Ti_3C_2T_x$ @MOF-303 achieves high pervaporation flux ($15.87\text{ kg m}^{-2}\text{ h}^{-1}$) with 99.84% NaCl rejection at 35°C [90], while UiO-66- NH_2 @MXene membranes increase water flux by >4 $\times$, reduce contact angle from 65° to 38°, and remove 72%–81% of cationic dyes and >91% of anionic dyes [47]. Advanced 3D-printed MXene/MOF lattices further enhance adsorption kinetics, surface accessibility, and recyclability, achieving >90% dye removal for methyl orange and direct red 31 [3, 35].

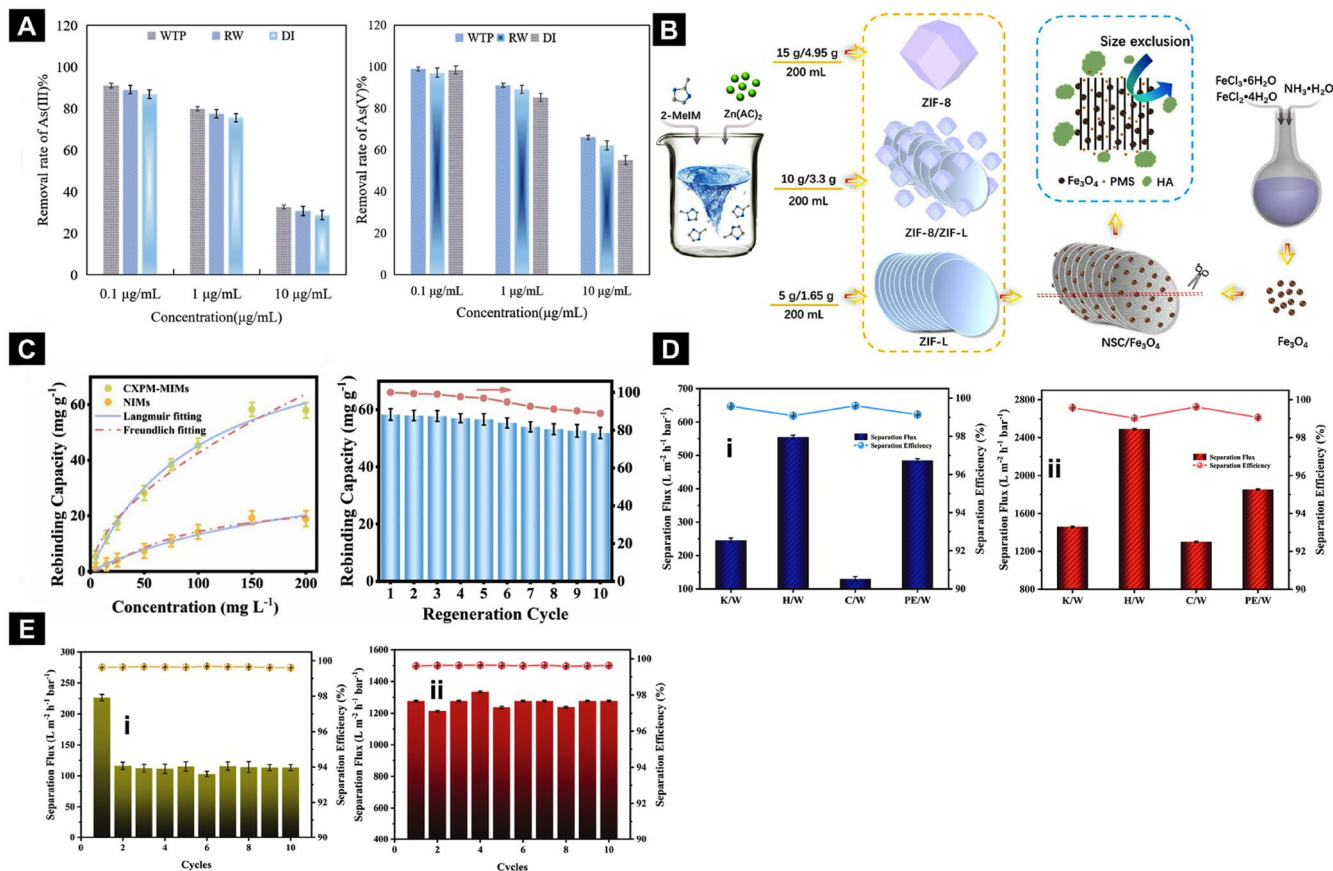


FIGURE 8 | (A) Heavy metal removal of As(III) and As(V) by Fe–ZIF-8@MXene. Reproduced from [84] with permission from MDPI. (B) Schematic illustration of NSC@Fe₃O₄ for PMS-activated tetracycline degradation. Reproduced from [80] with permission from Elsevier. (C) Isothermal adsorption of ribavirin on CXPM-MIMs and NIMs and regeneration stability for 10 cycles. Reproduced from [89] with permission from Elsevier. (D) Separation performance of (i) PEG/MXene and (ii) PEG/MXene@MOF membranes for kerosene-in-water (K/W), hexane-in-water (H/W), crude oil-in-water (C/W), and petroleum ether-in-water (PE/W) emulsions. (E) Cyclic stability of (i) PEG/MXene and (ii) PEG/MXene@MOF for C/W emulsion. Reproduced from [91] with permission from Elsevier.

5 | Challenges and Limitations

5.1 | Surface Oxidation and Degradation of MXenes

A primary challenge in the development of MXene–MOF hybrids is the inherent propensity of MXenes, particularly Ti₃C₂T_x, to undergo oxidation, thereby compromising their structural integrity (Figure 9A). Despite the exceptional conductivity and advantageous surface terminations of MXenes, which make them ideal candidates for adsorption and catalysis, these same properties render them highly reactive toward air, moisture, and dissolved oxygen [47]. The oxidation of MXenes at ambient temperature has been attributed to several factors, such as exposure to O₂, structural defects in as-synthesized MXenes, and functional clusters on the surface. Ghidui et al. observed the presence of oxygen-containing surface terminations and defect-rich regions on the Ti₃C₂T_x MXene surface, where the oxidized phase progressively permeates the layers, transforming the Ti–C structure into TiO₂, thereby inhibiting electron transfer and catalytic activity [131]. In another study, Habib et al. reported that Ti₃C₂T_x undergoes rapid oxidation in aqueous media within 2 weeks, resulting in 65% lower electrical conductivity relative to

the pristine sample [132]. Furthermore, the authors noted that exposure to UV light accelerated the oxidation of Ti₃C₂T_x films due to two factors: (i) the conversion of UV light to heat, which enhances oxidation kinetics because MXenes can absorb light and convert it to heat with 100% efficiency, and (ii) the generation of radicals from UV light, which can attack Ti₃C₂T_x and induce oxidation; prolonged UV exposure can lead to the formation of additional radicals, which exacerbate oxidation.

5.2 | Instability of MOFs in Aqueous Environments

Another challenge is that many MOFs do not perform well in aqueous environments. For example, MOFs constructed from carboxylate linkers and divalent metal centers, such as Zn²⁺, Cu²⁺, or Co²⁺, are particularly vulnerable to hydrolysis (Figure 9B). When water molecules enter the structure, they can break the metal–ligand bonds that hold the framework together, weakening or collapsing it over time [133]. This results in a loss of porosity and active sites, both of which are crucial for adsorption and catalytic performance. In the case of MXene–MOF hybrids, this becomes a serious problem because once the MOF

begins to break down, the MXene layers can restack and reduce the ability of the material to absorb pollutants or perform catalytic reactions. Al-Janabi et al. [134] reported that water molecules can significantly perturb the metal–ligand coordination of $\text{Cu}_3(\text{BTC})_2$ -based MOFs (HKUST-1). Partial displacement of the carboxylate groups of BTC ligands from open Cu sites was observed under dynamic water–vapor adsorption at 50°C, resulting in framework collapse and loss of porosity. The degradation of the structure was ascertained using small-angle X-ray scattering (SAXS), powder X-ray diffraction (PXRD), Fourier-transform infrared spectroscopy (FTIR), and differential scanning calorimetry (DSC) analyses, indicating that hydrolysis is a key limitation that hinders the application of MOFs in aqueous environments.

5.3 | Difficulty in Achieving Uniform Surface Interactions

Another significant challenge is achieving a stable and uniform interface between MXenes and MOFs (Figure 9C). The performance of the hybrid depends on the formation of strong and well-coordinated interactions across the interface, through Ti–O–M bonding, hydrogen bonding, or electrostatic forces. However, the surfaces of MXene are inconsistent due to variations in their surface terminations, defect densities, and partial oxidation states. These variations make it difficult to control the growth of MOFs on their surfaces. As a result, in situ growth methods often produce patchy or uneven MOF layers, particle clusters, or irregular crystal arrangements [135]. Ex-situ methods can be more unpredictable since the interactions involved are weaker, which increases the likelihood of detachment or non-uniform coverage. These inconsistencies ultimately affect the reliability of the hybrid and lead to fluctuating catalytic performance and inconsistent pollutant selectivity across batches. Liu et al. [136] reported that engineering a hydrogen-bonded interface between MXene and MOF can substantially improve cycling stability. This is because the weak coordination bonds of MOFs lead to structural instability and performance degradation. The introduction of quadruple hydrogen bonds (H-bonds) has been reported to enhance structural stability by forming cross-linked networks between molecules owing to the presence of multiple H-bonds. The authors also reported that the dynamic reversibility of hydrogen bonds provides the self-healing ability of MOFs, while the low binding energy compared to coordination bonds allows H-bonds to break preferentially when subjected to internal stress to protect the MOFs. Thus, interface engineering is a key bottleneck that should be addressed for the large-scale production of MXene–MOF hybrids.

5.4 | Environmental Safety and Catalytic By-Products

Although MXene–MOF hybrids are promising for pollutant removal, their environmental impact has not been fully understood. For instance, MOFs can degrade through hydrolysis and release metal ions and organic linkers into water. This can introduce new contaminants into the water system instead of eliminating existing pollutants (Figure 9D). Jastrzębska et al.

[137] reported cytotoxicity studies of Ti_3C_2 MXene on normal (MRC-5 and HaCaT) and cancerous (A549 and A375) cell lines, revealing more pronounced toxic effects in cancerous than in normal cells, and indicating that MXene can induce oxidative stress and the generation of reactive oxygen species (ROS). Nasrallah et al. [138] reported an ecotoxicological assessment of Ti_3C_2 MXene using a zebrafish embryo model. The authors reported that zebrafish embryos uptake Ti_3C_2 in a dose-dependent manner. Based on the sigmoidal mortality curve, the lowest-observed-effect concentration (LOEC; $\geq 20\%$ mortality) of MXene was reported to be $100\text{ }\mu\text{g mL}^{-1}$, with this concentration inducing a mortality of approximately 21%. Accordingly, the authors recommended the safe use and discharge of $\text{Ti}_3\text{C}_2\text{T}_x$ MXene at concentrations below $100\text{ }\mu\text{g mL}^{-1}$ in aquatic ecosystems. In a separate study, Bi et al. [139] investigated the influence of residual species on the catalytic degradation of aromatic volatile organic compounds (VOCs) using Pd catalysts supported on the Zr-based MOF UiO-66. The authors reported that residual Cl species from ZrCl_4 metal precursors were involved in the VOC degradation mechanism, which led to the generation of many by-products containing chlorine, including the hypertoxic dioxin precursor dichlorobenzene, which is environmentally persistent and raises concerns regarding secondary pollution during catalytic VOC treatment as well as significant environmental and health risks.

In addition, practical and economical constraints pose significant challenges for the large-scale production of MXene–MOF hybrids. For instance, common laboratory-scale techniques, such as in situ growth, layer-by-layer assembly, or vacuum-assisted membrane fabrication, require high reagent costs, prolonged processing duration, and specialized equipment, thereby limiting their economic feasibility. Moreover, the large-scale production of MXene–MOF hybrids requires precise control of reaction conditions to prevent oxidation and degradation of MXene and MOF, respectively, while ensuring homogenous and stable interfaces. Therefore, scalable, cost-effective, and reproducible synthesis strategies for MXene–MOF hybrids are necessary to facilitate their scale-up for practical applications in industrial wastewater treatment.

6 | Conclusion

Effective wastewater treatment is essential for safeguarding human health and preserving ecosystem integrity. MXene–MOF hybrids have emerged as promising materials for next-generation wastewater treatment, achieving high removal efficiencies (typically 90%–99%) for a wide range of pollutants through multiple mechanisms, including adsorption, photocatalysis, electrocatalysis, and membrane-based separation. Despite significant progress at the laboratory scale, several limitations still hinder the practical application of MXene–MOF hybrids in wastewater treatment. These limitations include scalability constraints, surface oxidation and degradation of MXenes, hydrolytic instability of MOFs in aqueous environments, difficulty in achieving uniform interfacial interactions, and the high cost of current synthesis routes. Hence, advances in green synthesis, robust interfacial engineering, and integration into application-relevant modules (e.g., membranes,

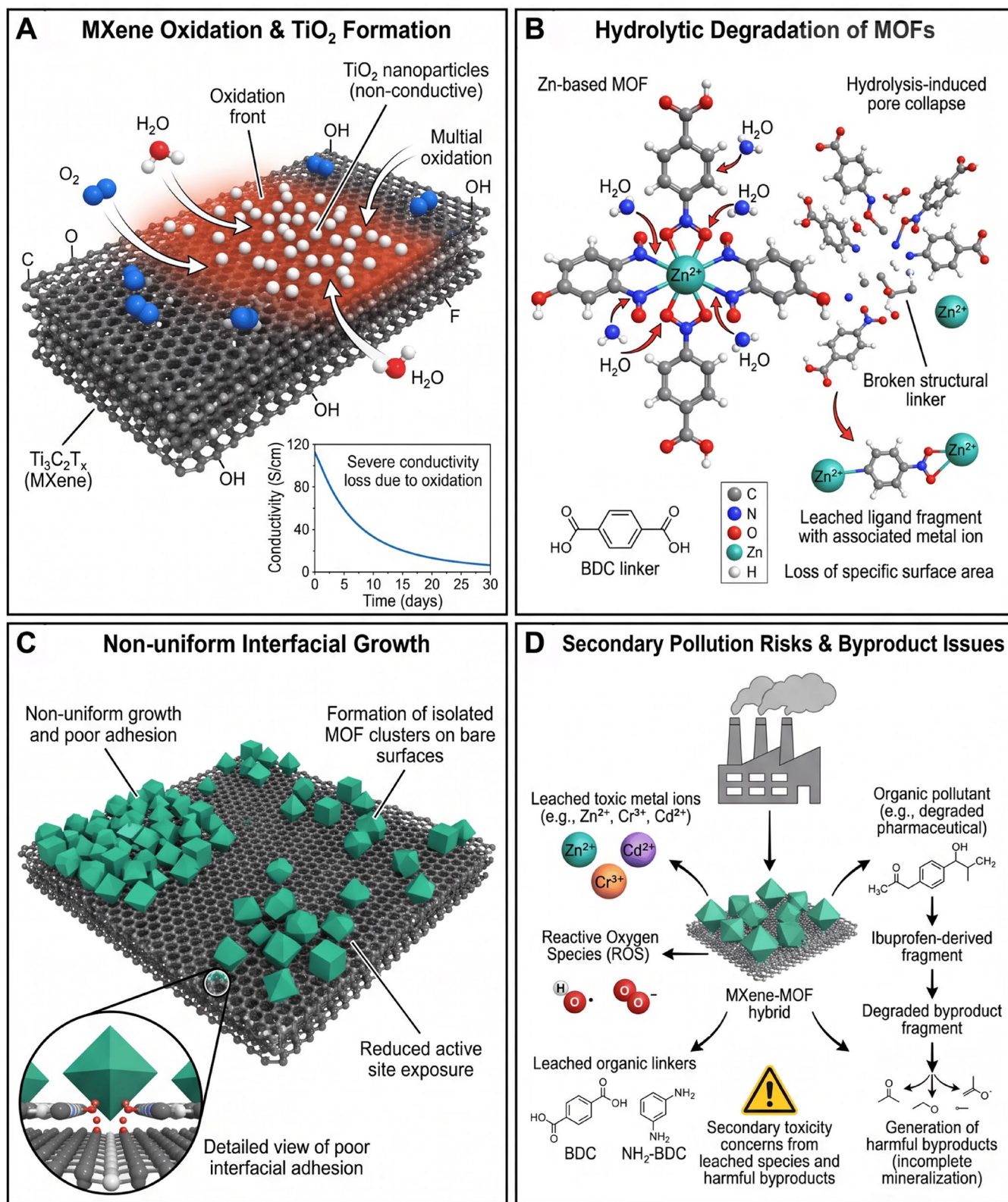


FIGURE 9 | Key challenges of MXene–MOF hybrids in wastewater treatment (A) oxidation of MXene ($\text{Ti}_3\text{C}_2\text{T}_x$) which causes TiO_2 formation, (B) hydrolytic degradation of MOFs, (C) non-uniform interfacial growth which causes poor adhesion and reduced exposure to active sites, (D) environmental concerns due to secondary pollution.

monoliths, and flow-through reactors) are crucial to provide a solid foundation for next-generation wastewater treatment technologies. With continued research and development,

MXene–MOF hybrids offer significant potential to enable more sustainable, efficient, and economically viable solutions to global wastewater treatment challenges.

Author Contributions

Kalaimani Markandan: conceptualization, methodology, literature review, data curation, formal analysis, visualization, project administration, writing – original draft preparation; **Theeba Rajasegran:** literature review, data curation, writing – review and editing; **Sharoen Lim Yu Ming:** literature review, data curation, writing – review and editing; **Santheraleka Ramanathan:** literature review, writing – review and editing; **Yong Wei Tiong:** literature review, writing – review and editing; **Thachnatharen Nagarajan:** formal analysis, visualization, writing – review and editing; **Mohammad Khalid:** conceptualization, methodology, supervision, writing – review and editing. All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest

The authors declare no conflicts of interest.

Data Availability Statement

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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